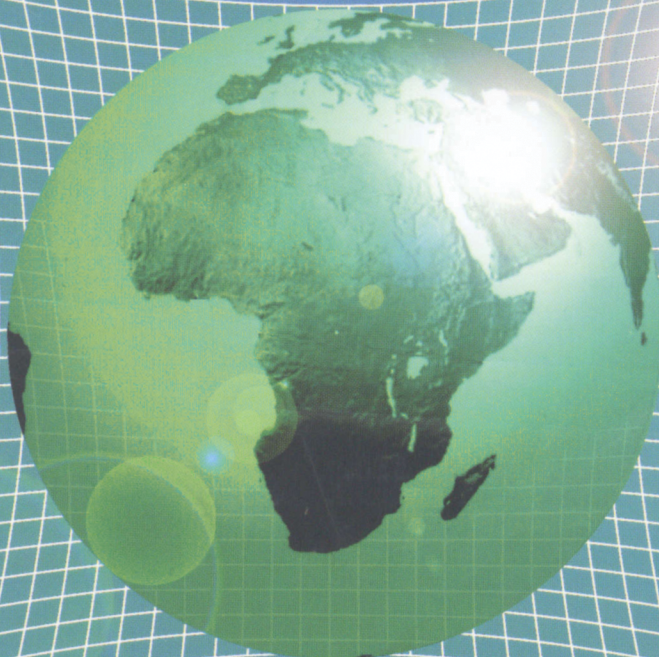


The Dictionary of Substances and their Effects

Second Edition

Editor
Sharat Gangolli



Volume 7
T-Z and Index

**The Dictionary
of Substances
and their Effects**
Second Edition

The Dictionary of Substances and their Effects

Second Edition

EDITOR

S Gangolli, *Consultant, MRC Toxicology Unit, UK*

EDITORIAL ADVISORY BOARD

Dr D Anderson, *BIBRA International, UK*

Dr J Chadwick, *Health and Safety Executive, UK*

Professor L Ebdon, *University of Plymouth, UK*

Dr D Gammon, *California EPA, USA*

Professor L King, *University of Surrey, UK*

Dr R McClellan, *Chemical Industry Institute of Toxicology, USA*

Professor I Rowland, *University of Ulster, UK*

Dr J Solbé, *Unilever, UK*

Dr T Sugimura, *National Cancer Centre, Japan*

Professor P van Bladeren, *TNO Nutrition and Food Research Institute, The Netherlands*

PRODUCTION TEAM

Ken Wilkinson (Staff Editor)
Richard Ellis
Sally Faint
Julie Hetherington
Alan Skull

The publishers make no representation, express or implied, with regard to the accuracy of the information contained in this book and cannot accept any legal responsibility or liability for any errors or omissions that may be made.

Volume 7 ISBN 0-85404-838-3
Seven-volume set ISBN 0-85404-803-0

A catalogue record for this book is available from the British Library.

© The Royal Society of Chemistry 1999

All rights reserved

Apart from any fair dealing for the purpose of research or private study, or criticism or review as permitted under the terms of the UK Copyright, Designs and Patents Act, 1988, this publication may not be reproduced, stored or transmitted, in any form or by any means, without the prior permission in writing of The Royal Society of Chemistry, or in the case of reprographic reproduction only in accordance with the terms of the licences issued by the Copyright Licensing Agency in the UK, or in accordance with the terms of the licences issued by the appropriate Reproduction Rights Organisation outside the UK. Enquiries concerning reproduction outside the terms stated here should be sent to The Royal Society of Chemistry at the address printed on this page.

Published by The Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK

Typeset by Land & Unwin (Data Sciences) Ltd, Bugbrooke, UK

Printed and bound by Bookcraft (Bath) Ltd., UK

Contents

Volume 1

Foreword	vii
Introduction	ix
Guide to Content	xi
A-B Compounds	1–862
Abbreviations	863–865
Glossary of Medical and Biological Terms	867–881
Glossary of Organism Names	882–889

Volume 2

Guide to Content	vii
C Compounds	1–865

Volume 3

Guide to Content	vii
D Compounds	1–832

Volume 4

Guide to Content	vii
E-J Compounds	1–892

Volume 5

Guide to Content	vii
K-N Compounds	1–953

Volume 6

Guide to Content	vii
O-S Compounds	1–952

Volume 7

Guide to Content	vii
T-Z Compounds	1–712
Index of Chemical Names and Synonyms	713–914
Index of CAS Registry Numbers	915–956
Index of Molecular Formulae	957–998

Guide to Content

The data for each chemical in DOSE are organised as follows:

DOSE No.
Chemical name
Structure/line formula
Molecular formula
Molecular weight
CAS Registry No.
Synonyms
EINECS No.
RTECS No.
Uses
Occurrence

Physical properties

Melting point
Boiling point
Flash point
Specific gravity
Partition coefficient
Volatility
Solubility

Occupational exposure

Limit values
UN number
HAZCHEM code
Conveyance classification
Supply classification
Risk phrases
Safety phrases

Ecotoxicity

Fish toxicity

Invertebrate toxicity
Toxicity to other species
Bioaccumulation

Environmental fate

Nitrification inhibition
Carbonaceous inhibition
Anaerobic effects
Degradation studies
Abiotic removal
Adsorption and retention

Mammalian and avian toxicity

Acute data
Sub-acute and sub-chronic data
Carcinogenicity and chronic effects
Teratogenicity and reproductive effects
Metabolism and toxicokinetics
Irritancy
Sensitisation

Genotoxicity

Other effects

Other adverse effects (human)
Any other adverse effects

Legislation

Other comments

References

These headings only appear in an item when data have been identified for that heading. The user can, therefore, assume that the absence of a heading means that no relevant data were retrieved from the sources examined.

Dose No.

Each of the 4123 compounds in DOSE is identified by a unique, sequential alphanumeric DOSE No. For example, the first compound in DOSE, *A- α -C*, has DOSE No. *A1*; the last entry, *zoxazolamine*, has DOSE No. *Z25*.

Chemical name

In general, the chemical name is the common name of the substance, for example *nitrobenzene*. If it is not possible to allocate a precise chemical name (i.e. if the substance is of unknown or variable composition, or consists of biological materials), a short phrase appears instead, for example *chlorinated paraffins (C12, 60%)*.

Molecular formula

This is the elemental composition of the compound. The elements appear alphabetically for inorganic compounds, i.e. Ag_2CO_3 , Cl_2Cr , etc, but for organic compounds, carbon and hydrogen content are shown first followed by the other elements in alphabetical order, i.e. $\text{C}_6\text{H}_5\text{Br}$.

Molecular weight

This is directly calculated from the molecular formula. No molecular weights are given for polymers.

CAS Registry No.

The CAS Registry No. is a number sequence adopted by the Chemical Abstracts Service (American Chemical Society, Columbus, Ohio, USA) to uniquely identify specific chemical substances. The number contains no information relating to the chemical structure of a substance and is, in effect, a catalogue number relating to one of the millions of unique chemical substances recorded in the CAS Registry. New numbers are assigned sequentially to each new compound identified by Chemical Abstracts Service. This information is also provided in the full index of CAS Registry Numbers available at the end of Volume 7.

Synonyms

For common chemicals, several chemical names and numerous trade names may be applied to describe the chemical in question. Many of these names are identified to aid users on the range of names which have been used to describe each substance.

EINECS No.

This number is assigned by the European Commission to each record in the EINECS (European Inventory of Existing Commercial Chemical Substances) inventory. The numbers are in the format XXX-XXX-X, for example, *202-716-0* for *nitrobenzene*.

RTECS No.

The RTECS (Registry of Toxic Effects of Chemical Substances) number is a unique identifier assigned by NIOSH (National Institute of Occupational Safety and Health in the US) to every substance in the RTECS database. The number is in the format of two alphabetic characters followed by seven numeric characters, for example, *DA 6475000* for *nitrobenzene*.

Uses

Principal uses of the substances are given, with information on other significant uses in industrial processes.

Occurrence

Natural occurrences, whether in plants, animals or fungi are reported.

Physical properties

Melting/Boiling point

These data are derived from various sources.

Flash point

The flash point is the lowest temperature at which the vapours of a volatile combustible substance will sustain combustion in air when exposed to a flame. The flash point information is derived from various sources. Where possible the method of determination of the flash point is given.

Specific gravity (density)

The specific gravity of each substance has been derived from a variety of sources. Where possible the data have been standardised.

Partition coefficient

Partition coefficients, important for structure-activity relationship considerations, particularly in the aquatic environment, are indicated. Ideally the *n*-octanol/water partition coefficient is quoted. The major data source for this measurement is:

Sangster, J J. *Phys. Chem. Ref. Data* 1989, **18**(3), 1111-1229

Where no reference is quoted, it can be assumed that the information was derived from this source.

Volatility

The vapour pressure and vapour density are quoted where available. Where possible, the data have been standardised.

Solubility

Solubility data derived from several sources are quoted for both water and organic solvents where available.

Occupational exposure

Limit values

This field contains the occupational exposure limit values (or threshold limit values) from France, Germany, Japan, Sweden, UK and USA.

The airborne limits of permitted concentrations of hazardous chemicals represent conditions under which it is believed that nearly all workers may be repeatedly exposed day after day without adverse effect. These limits are subject to periodic revision and vary between different countries. The term *threshold limit* relates primarily to the USA, but equivalent terms are available in most industrialised countries. The data relates to concentrations of substances expressed in *parts per million (ppm)* and *milligrams per cubic meter (mg m⁻³)*.

French exposure limits are published by the French Ministry in Charge of Labour and presented in the report *Valeurs limites d'exposition professionnelle aux agents chimiques en France* (ND 1945-153-93). The values in DOSE have been taken from the 1998 edition. The FR-VLE values are short-term limits (15 minutes), and FR-VME values are long-term limits (8 hours).

German data currently include the national MAK values where available. The MAK value (Maximale Arbeitsplatz-Konzentration) is defined as the maximum permissible concentration of a chemical compound present in the air within a working area which, according to current knowledge, does not impair the health of the employee or cause undue annoyance. Under those conditions, exposure can be repeated and of long duration over a daily period of eight hours, constituting an average working week of 40 hours. MAK values are published by the Geschäftsstelle der Deutschen Forschungsgemeinschaft, Bonn, in "Maximum Concentrations at the Workplace and Biological Tolerance Values for Working Materials." The values in DOSE have been taken from the 1998 edition.

Japanese exposure limits are those recommended by the Japanese Society of Occupational Health. Unless otherwise indicated, these values are long-term exposure limits (the mean exposure concentration at or below which adverse health effects caused by the substance do not appear in most workers, working 8 hours a day, 40 hours a week under a moderate workload). The values in DOSE were published in 1997.

Swedish data can include short-term exposure limit, a level limit, or a ceiling limit. The values in DOSE were adopted in 1996.

In the UK occupational limits relating to airborne substances hazardous to health are published by the Health and Safety Executive annually in Guidance Note EH40. The values in the DOSE items have been taken from the 1999 edition.

There are Maximum Exposure Limits (MEL) in the UK which are subject to regulation and which should not normally be exceeded. They derive from Regulations, Approved Codes of Practice, European Community Directives, or from the Health and Safety Commission. In addition, there are Occupational Exposure Standards (OES) which are considered to represent good practice and realistic criteria for the control of exposure. In an analogous fashion to the USA Threshold Limits, there are long-term limits, expressed as time-weighted average concentrations over an 8-hour working day, designed to protect workers against the effects of long-term exposure. The short-term exposure limit is for a time-weighted average of 15 minutes. For those substances for which no short-term limit is listed, it is recommended that a figure of three times the long-term exposure limit averaged over a 15-minute period be used as a guideline for controlling exposure to short-term excursions.

The threshold limit values for the USA have been taken from the *Threshold Limit Values and Biological Exposure Indices, 1999* produced by the American Conference of Governmental Industrial Hygienists, Cincinnati, USA. The limits relate to *Threshold Limit – Time Weighted Average*, *Threshold Limit – Short Term Exposure Limit* and *Threshold Limit – Ceiling Limit*. The Threshold Limit Value – Time Weighted Average (TLV-TWA) allows a time-weighted average concentration for a normal 8-hour working day and a 40-hour working week, to which nearly all workers may be repeatedly exposed day after day, without adverse effect. The Threshold Limit Value – Short Term Exposure Limit (TLV-STEL) is defined as a 15-minute, time-weighted average which should not be exceeded at any time during a work day, even if the 8-hour time-weighted average is within the TLV. It is designed to protect workers from chemicals which may cause irritancy, chronic or irreversible tissue damage, or narcosis of sufficient degree to cause the likelihood of accidental injury. Many STELs have been deleted pending further toxicological assessment. With Threshold Limit – Ceiling Values (TLV-C) the concentration should not be exceeded during any part of the working day.

UN number

The United Nations Number is a four-figure code used to identify hazardous chemicals and is used for identification of chemicals transported internationally by road, rail, sea and air. In the UK this number is also called the “Substance Identification Number” or “SI Number”.

HAZCHEM code

The Hazchem Code is used to instruct United Kingdom emergency services on equipment, evacuation and other methods of dealing with transportation incidents. It is administered by the Chemical Industries Association.

Conveyance classification

The information presented for the transportation of substances dangerous for conveyance by road is derived from the UK’s Approved Carriage List, Health and Safety Commission, UK.

Supply classification

The information presented for the supply of substances is derived from the UK’s Approved Supply List: information approved for the classification and labelling of substances and preparations dangerous for supply [Chemicals (Hazard Information and Packaging) Regulations 1999 (CHIP 99)*] Health and Safety Commission, UK.

Risk and safety phrases

Risk and safety phrases used in connection with DOSE items are approved phrases for describing the risks involved in the use of hazardous chemicals and have validity in the United Kingdom and throughout the countries of the European Community. The approved texts have designated R (Risk) and S (Safety) numbers from which it is possible to provide translations for all approved languages adopted by the European Community. The risk and safety phrases quoted in DOSE relate to the UK’s Approved Supply List: information

*At the time of going to press the Health and Safety Commission, UK announced that an amendment (Amendment No. 2) to the CHIP 99 regulations is intended to come into force on 1 January 2000. The supply classifications and the risk and safety phrases reported in this edition of DOSE do not include any changes which are proposed in Amendment No. 2 to CHIP 99. These changes are incorporated in the updates to the electronic versions of DOSE released after 1 January 2000.

approved for the classification and labelling of substances and preparations dangerous for supply [Chemicals (Hazard Information and Packaging) Regulations, 1999 (CHIP 99)] Health and Safety Commission, UK. The risk and safety phrases should be used to describe the hazards of chemicals on data sheets for use and supply; for labelling of containers, storage drums, tanks etc., and for labelling of articles specified as dangerous for conveyance by road. (See also footnote on page xi.)

Ecotoxicity

Information is presented on the effects of chemicals on various ecosystems. Results of studies carried out on aquatic species, primarily fish and invertebrates, but also fresh water and marine microorganisms and plants are reported. Persistence and potential for accumulation in the environment and any available information on the harmful effects to non-target species, i.e. the unintentional exposure of terrestrial and/or aquatic species to a toxic substance is given. Ecotoxicology can be defined as that science involved in the study of the production of harmful effects by substances entering the natural environment, especially effects on populations, communities and ecosystems; or as the study of the effects of chemicals on ecosystems and their non-human components. An essential part of the ecotoxicology is the assessment of movement of potentially toxic imbalance through environmental compartments and through food webs.

Ecotoxicology, unlike human toxicology, is more concerned with the effects to populations than to individuals. Human toxicology is based on the extrapolation of data from many species to one species man, whereas ecotoxicology necessitates the extrapolation from a few species to many, or from limited field data to entire ecosystems.

Ecotoxicology must not be confused with environmental toxicology which is the direct effects of environmental chemicals to humans. The term environmental toxicology should only be applied to the study of direct effects of environmental chemicals on human beings. Although the main thrust of preventative toxicology is in the area of human health, it is becoming increasingly evident that human health is intimately connected with conditions in the natural environment. Chemicals released into the environment far from human habitation may become a health hazard for humans through food chain accumulation. Other chemicals may adversely affect crop growth or kill economically important fish stocks or bird life.

Fish toxicity

LC₅₀ values, with duration of exposure, are quoted for two species of freshwater and one marine species if available. Any additional information on bioassay type (static or flow through) and water condition (pH, temperature, hardness or oxygen content) is reported.

Invertebrate toxicity

LC₅₀ values with duration of exposure, are quoted for molluscs and crustaceans. EC₅₀ values, i.e. concentrations which will immobilise 50% of an exposed population, are given for microbes, algae and bacteria. Values which will inhibit microbial or algal growth are reported. Duration of exposure is given when available.

Toxicity to other species

Toxicity to species other than mammals, birds, invertebrates and fish (e.g. reptiles, amphibians, plants, seaweeds), is reported here. LD₅₀, LC₅₀ and EC₅₀ values are given with duration of exposure, concentration and as much supplementary information as possible.

Bioaccumulation

Bioaccumulation, biomagnification and bioconcentration data are quoted primarily for fish, invertebrates, bacteria and algae. Bioaccumulation is the progressive increase in the amount of a chemical in an organism or part of an organism which occurs because the rate of intake exceeds the organism's ability to remove the substance from its body. Bioconcentration is a process leading to a higher concentration of a chemical in an organism than in its environment. Lastly, biomagnification is a sequence of processes in an ecosystem by which higher concentrations are attained in organisms at higher trophic levels, i.e. at higher levels in the food chain.

Environmental Fate

Degradation data are used to assess the persistence of a chemical substance in the environment, in water, soil and air. If the substance does not persist, information on the degradation products is also desirable. Intermediates may be either harmless or toxic substances which will themselves persist. Degradation occurs via two major routes, microbial degradation utilising microorganisms from a variety of habitats and decomposition by chemical methods. Microbial degradation is associated with the production of elemental carbon, nitrogen and sulfur from complex molecules. Standard biodegradation tests estimate the importance of microbial biodegradation as a persistence factor. Most tests use relatively dense microbial populations adapted to the compound being studied. Rapid degradation results in these tests implies that the compound will degrade under most environmental conditions, although specialised environments where degradation would not occur can exist. Compounds which are not readily degradable are likely to persist over a wide range of environmental situations.

Chemical degradation processes include photolysis, hydrolysis, oxidation and removal by reversible/irreversible binding to sediment. Factors which influence degradation rates, such as duration of exposure, temperature, pH, salinity, concentrations of test substance, microbial populations, and other nutrients, must also be taken into account.

Due care must also be given when metabolism results in the production of substances that are more toxic than their parents.

Nitrification inhibition

The nitrogen cycle is the major biogeochemical process in the production of nitrogen, an essential element contained in amino acids and proteins. Nitrogen is an essential element in microorganisms, higher plants and animals. Interference in the production of nitrogen from more complex molecules can be determined by standard tests using nitrogen-fixing bacteria. The degree of inhibition can be used to estimate the environmental impact of the test chemical.

Carbonaceous inhibition

Another major biogeochemical process is the recycling of carbon via the decomposition of complex organic matter by bacteria and fungi. In nature the process is important in the cycling of elements and nutrients in ecosystems. The degradation sequence occurs in stages, cellulose → cellobiose → glucose → organic acids and carbon dioxide. Chemical inhibition of microbial processes at all or any of these stages is reported here.

Anaerobic effects

Anaerobic microbial degradation of organic compounds occurs in the absence of oxygen and is an important degradation process in both the natural environment and in waste treatment plants. Data on the effects of chemicals on anaerobic systems are reported here. An important method uses anaerobic digestion tests which compare the production of methane and carbon dioxide by anaerobic microbes in a sludge sample with and without added test material. Methane production is at the end of the food chain process used by a wide range of anaerobic microorganisms.

Degradation studies

This section focuses on microbial degradation in both soil and water under anaerobic and aerobic conditions. The half-life of the chemical substance in the environment is reported with its degradation products where possible, giving an indication of the degree of its persistence. Water pollution factors: BOD (biochemical/biological oxygen demand), COD (chemical oxygen demand) and ThOD (theoretical oxygen demand) are stated, where available. BOD estimates the extent of natural purification which would occur if a substance were discharged into rivers, lakes or the sea. COD is a quicker chemical method for this determination which uses potassium dichromate or permanganate to establish the extent of oxidation likely to occur. ThOD measures the amount of oxygen needed to oxidise hydrocarbons to carbon dioxide and water. When organic molecules contain other elements nitrogen, sulfur or phosphorus, the ThOD depends on the final oxidation stage of these elements.

Abiotic removal

Information on chemical decomposition processes is contained in this section. The energy from the sun is able to break carbon-carbon, and carbon-hydrogen bonds, cause photodissociation of nitrogen dioxide to nitric oxide and atomic oxygen and photolytically produce significant amounts of hydroxyl radicals. Hydrolysis occurs when a substance present in water is able to react with the hydrogen or hydroxyl ions of the water. Therefore the extent of photolytic and oxidative reactions occurring in the atmosphere and hydrolysis in water can be used as a measure of environmental pollution likely to arise from exposure to a substance. Removal by activated carbon is also reported.

Adsorption and retention

The environmental impact of a chemical substance is determined by its ability to move through the environment. This movement depends on the affinity of the chemical toward particulate matter: soil and sediment. Chemicals which have a high affinity for adsorption are less readily transported in the gaseous phase or in solution, and therefore can accumulate in a particular medium. Chemical substances which are not readily adsorbed are transported through soil, air and aquatic systems.

Mammalian and avian toxicity

Studies on mammalian species are carried out to determine the potential toxicity of substances to humans. Avian species are studied primarily to assess the environmental impact on the ecosystem, however data from avian studies are also used for assessing human toxicity. This is specifically applied to pesticides, with neurotoxicology studies.

Procedures involve undertaking a series of established exposure studies on a particular substance using specific routes, oral, inhalation, dermal or injection for variable durations. Exposure durations include acute or single exposure to a given concentration of substance. Sub-acute or sub-chronic exposure, i.e. repeat doses over an intermediate time period, up to 4 weeks for sub-acute and 90 day/13 week (in rodents) or 1 year (in dogs) for sub-chronic studies. Chronic/long-term studies involve exposure to specific concentrations of chemical for a duration of 18 month-2 years. A variety of species are used in toxicity testing, most commonly rodents (rats, mice, hamsters) and rabbits, but tests can also be carried out on monkeys, domestic animals and birds.

Acute data

Single exposure studies quoting LD₅₀, LC_{LO}, LD_{LO}, TC_{LO} and TD_{LO} data.

Sub-acute and sub-chronic data

Results of repeat doses, intermediate duration studies are quoted. Priority is given to reporting the adverse effects on the gastro-intestinal, hepatic, circulatory, cardiopulmonary, immune, renal and central nervous systems.

Carcinogenicity and chronic effects

Information on the carcinogenicity of substances unequivocally proven to cause cancer in humans and laboratory animals, together with equivocal data from carcinogenicity assays in laboratory animals are reported. Additionally, treatment-related chronic adverse effects are reported. Criteria for inclusion required the study to report the species, duration of exposure, concentration and target organ(s); sex is also given where available.

Teratogenicity and reproductive effects

The results of studies carried out in intact animal and *in vitro* systems to determine the potential for teratogenic, foetotoxic and reproductive damage are reported here. Criteria for inclusion required the species, duration of exposure, concentration and details of the effect in relation to fertility to be stated. Adverse effects reported in this section include sexual organ dysfunction, developmental changes (to embryos and foetuses), malformations, increases in spontaneous abortions or stillbirths, impotence, menstrual disorders and neurotoxic effects on offspring.

Metabolism and toxicokinetics

Data are quoted on the metabolic fate of the substance in mammals, and includes adsorption, distribution, storage and excretion. Mechanisms of anabolic or catabolic metabolism, enzyme activation and half-lives within the body are reported when available. Additionally findings from *in vitro* studies are reported.

Irritancy

Chemical substances which cause irritation (itching, inflammation) to skin, eye and mucous membranes on immediate contact in either humans or experimental animals are reported here. Exposure can be intentional in human or animal experiments, or unintentional via exposure at work or accident to humans.

Sensitisation

Sensitisation occurs where an initial accidental or intentional exposure to a large or small concentration of substance causes no reaction or irritant effects. However, repeat or prolonged exposure to even minute amounts of a sensitising chemical causes increasingly acute allergic reactions.

Genotoxicity

Genotoxicity testing is carried out to determine the mutagenic and/or carcinogenic potential of a chemical substance. A standard series of tests are carried out under controlled laboratory conditions on an established set of test organisms. A hierarchical system using bacteria, yeasts, cultured human and mammalian cells, *in vivo* cytogenetic tests in mammals and plant genetics is used to assess the genotoxic potential of the substance under study. Bacteria, unlike mammals, lack the necessary oxidative enzyme systems for metabolising foreign compounds to the electrophilic metabolites capable of reacting with DNA. Therefore, bacteria are treated with the substance under study in the presence of a post-mitochondrial supernatant (S9) prepared from the livers of mammals (usually rats). This fraction is supplemented with essential co-factors to form the S9 mix necessary for activation. DOSE reports published studies: giving the test organisms, whether metabolic activation (S9) was required, and the result, positive or negative.

Other effects

Other adverse effects (human)

Adverse effects to humans from single or repeat exposures to a substance are given. The section includes results of epidemiological studies, smaller less comprehensive studies of people exposed through their work environment and accidental exposure of a single, few or many individuals.

Any other adverse effects

Adverse effects to organisms or animals other than man are reported here.

Legislation

Any form of legislation, medical (food and drugs) or environmental from European, American and worldwide sources is reported.

Other comments

All other relevant information, including chemical instability and incompatibility, reviews, phytotoxicity and toxic effects associated with impurities, is contained in this section.

References

Contains references to data from above sections.

Indexes

The most convenient means of accessing a chemical in DOSE is via one of the indexes at the back of Volume 7. DOSE contains three indexes: chemical name and synonyms, CAS Registry Numbers and molecular formulae.

Index of chemical names and synonyms

Contains the name of the chemical used in DOSE together with a number of synonyms for that chemical. All names are arranged alphabetically.

Index of CAS Registry Numbers

Contains a list of the CAS Registry Numbers of the chemicals in DOSE in ascending order. This number is linked to the preferred DOSE name for that chemical and its DOSE number.

Index of molecular formulae

Contains a list of the molecular formulae of the chemicals in DOSE in alphabetical order for inorganic compounds, i.e. Ag_2CO_3 , Cl_2Cr , etc., but for organic compounds, carbon and hydrogen content are shown first followed by the other elements in alphabetical order, i.e. $\text{C}_6\text{H}_5\text{Br}$. This number is linked to the preferred DOSE name for that chemical and its DOSE number.

Note

The Royal Society of Chemistry (RSC) has only assessed published information in compiling The Dictionary of Substances and their Effects. However, the RSC would welcome any relevant information on the chemicals that is not readily accessible, but in the public domain, for inclusion when the items in DOSE are updated.

If you have any relevant information, please contact:

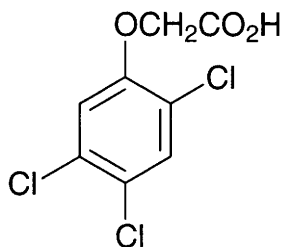
Chemical Databank Production
Royal Society of Chemistry
Thomas Graham House
Science Park
Cambridge CB4 0WF
UK
Telephone: +44 (0)1223 420066
Fax: +44 (0)1223 423429

Document Delivery

The Library and Information Centre (LIC) of the RSC offers a Document Delivery Service for items in chemistry and related subjects. Contact: Library and Information Centre, the Royal Society of Chemistry, Burlington House, Piccadilly, London W1V 0BN, UK.

Telephone: +44 (0)20 7437 8656
Fax: + 44 (0)20 7287 9798
Email: library@rsc.org

T1 2,4,5-T



$C_8H_5Cl_3O_3$

Mol. Wt. 255.48

CAS Registry No. 93-76-5

Synonyms 2,4,5-trichlorophenoxyacetic acid; acetic acid, (2,4,5-trichlorophenoxy)-; Dacamine; Ded-weed; Forron; T-Nox; U46

EINECS No. 202-273-3

RTECS No. AJ 8400000

Uses Superseded herbicide.

Physical properties

M. Pt. 153-156°C **Specific gravity** 1.80 at 20°C with respect to water at 20°C

Partition coefficient $\log P_{ow}$ 3.00 (calc.) (1) **Volatility** v.p. 6.46×10^{-6} mmHg at 25°C

Solubility Water: 150 mg l⁻¹ at 25°C. Organic solvents: diethyl ether, ethanol, toluene

Occupational exposure

DE-MAK 10 mg m⁻³ (inhalable fraction of aerosol)

FR-VME 10 mg m⁻³

UK-LTEL 10 mg m⁻³

UK-STEL 20 mg m⁻³

US-TWA 10 mg m⁻³

Supply classification harmful, dangerous for the environment

Risk phrases Harmful if swallowed – Irritating to eyes, respiratory system and skin – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R22, R36/37/38, R50/53)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with the skin – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S24, S60, S61)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) rainbow trout, carp 350, 355 mg l⁻¹, respectively (2).

LC₅₀ (96 hr) perch, guppy 16.4, 28.1 mg l⁻¹, respectively (3).

Invertebrate toxicity

EC₅₀ (5 min) *Photobacterium phosphoreum* 52-158 ppm Microtox test (4).

LC₅₀ (96 hr) *Daphnia magna* 55 mg l⁻¹ (5).

EC₅₀ (10 day) *Isochrysis galbana*, *Phaeodactylum tricornutum* 50 mg l⁻¹ (6).

Bioaccumulation

Mosquito fish bioconcentration factor 264 after 32 days (7).

American coot residue concentrations in breast muscle 199 ppb, fat 21 ppb, and liver 39 ppb (8).

Environmental fate

Degradation studies

The herbicide was dehalogenated in samples from a methanogenic aquifer to form 2,4- and 2,5-dichlorophenoxyacetic acids; further incubation produced several intermediates, including mono- and dichlorophenol, monochlorophenoxyacetic acids and phenol. The pattern of intermediate formation suggests the anaerobic degradation proceeded by a series of dehalogenation steps, with side-chain cleavage reactions occurring before ring cleavage (9).

>205 days for ring cleavage in a soil suspension (10).

75-100% disappears from soil in 5 months (11).

Mammalian & avian toxicity

Acute data

LC₅₀ (8 day) oral bobwhite quail, mallard duck 2776, >4650 mg kg⁻¹ in diet, respectively (12).

LD₅₀ oral rat, mouse 300-390 mg kg⁻¹ (12).

LD₅₀ dermal rat >5000 mg kg⁻¹ (12).

LD₅₀ dermal rat 1535 mg kg⁻¹ (13).

Sub-acute and sub-chronic data

In 90-day feeding trials no effects were observed in dogs receiving 60 mg kg⁻¹ diet (12).

Oral dogs (14-day study) received single doses of 50, 100, 250 or 400 mg kg⁻¹; the numbers of deaths were 0/4, 1/4, 1/1 and 1/1, respectively. The animals suffered only weight loss, slight to moderate stiffness in the hind legs and ataxia (at the highest dose) (14).

Oral rat (3 wk) 20, 100 or 250 mg kg⁻¹ day⁻¹. Even at the lowest dose the herbicide caused a significant decrease in relative kidney weight and a significant increase in serum IgG. The LOEC was set at 20 mg kg⁻¹ day⁻¹ (15).

Oral dog (13 wk) 0, 2, 5, 10 or 20 mg kg⁻¹ 5 day wk⁻¹. No deaths occurred at ≤10 mg kg⁻¹ day⁻¹ diet. No effects on body weight, haematology and pathology were seen except in animals that died. The NOEL level was set at 10 mg kg⁻¹ day⁻¹ (14).

Carcinogenicity and chronic effects

There were inadequate data regarding carcinogenicity to animals to allow an IARC classification to be made (16).

In 2-yr feeding trials no effects were observed in rats receiving 30 mg kg⁻¹ diet (12).

Oral ♂, ♀ rats (2 yr) 3, 10 or 30 mg kg⁻¹ day⁻¹. There was no significant increase in tumour incidence in any treated group compared with control animals. At the highest dose there was a decrease in body weight and an increase in relative kidney weight. Increases in the volume of urine excreted and increased morphological changes in the liver, kidney and lungs were also seen at this dose. At 10 mg kg⁻¹ an increased incidence of mineralised deposits in the renal pelvis of ♀ was noted. At 3 mg kg⁻¹ there were no changes that were considered to be treatment related (17).

Teratogenicity and reproductive effects

Gavage mouse (days 8-12 of gestation) classified as a teratogen by the Chernoff/Kavlock developmental toxicity screen (18).

Oral Rhesus monkey (days 22-38 of gestation) 0.05, 1.0 or 10 mg kg⁻¹ day⁻¹. No toxicity was seen in the mothers and no teratogenic effects were observed in offspring (19).

Gavage rats (days 6-15 of gestation) 1, 3, 6, 12 or 24 mg kg⁻¹ day⁻¹ and oral rabbit (days 6-18 of gestation) 10, 20 or 40 mg kg⁻¹ day⁻¹. No observable effects were seen in dams of either species and litter size, number of foetal resorptions, birth weights and sex ratios were unaffected. No embryotoxic or teratogenic effects were seen after detailed visceral and skeletal examinations (20).

Oral mice (days 15-16 gestation) 0, 20, 35, 60, 90 or 100 mg kg⁻¹ day⁻¹. Foetal weight was significantly lower than controls at all doses. Resorptions were significantly increased at ≥60 mg kg⁻¹ and the incidence of cleft palates was higher at ≥35 mg kg⁻¹; no effects were seen at 20 mg kg⁻¹ (21).

Metabolism and toxicokinetics

Gavage ♂ rat single dose of 50 mg kg⁻¹. 45-70% of the dose was recovered in urine within 7 days (22).

Oral ♂ humans single dose of 5 mg kg⁻¹. Almost all the compound was excreted unchanged via the urine,

indicating that gastro-intestinal absorption was nearly complete and that little metabolism occurred; no clinical effects were seen in the volunteers (23).

Gavage ♀ rats (including pregnant animals) 0.17, 4.3 or 41 mg kg⁻¹ ¹⁴C-labelled compound. In the first 24 hr, 75 ± 7% of the radioactivity was excreted in urine and 8.2% was excreted in the faeces; no ¹⁴C was found in expired air (24).

Irritancy

The dry material is slightly irritating to the skin and eyes of animals. The highly concentrated solution may burn the skin with repeated or prolonged contact and can strongly irritate the eyes and possibly cause corneal damage (25).

Genotoxicity

Salmonella typhimurium SV50 with and without metabolic activation negative (26).

Escherichia coli PQ37 SOS-chromotest with and without metabolic activation negative (27).

In vitro Chinese hamster ovary cells sister chromatid exchanges with and without metabolic activation positive, chromosomal aberrations with metabolic activation positive (28).

Saccharomyces cerevisiae mitotic gene conversion negative (29).

In vivo mouse bone marrow cells did not induce micronuclei (30).

Other effects

Other adverse effects (human)

Following an explosion at a chemical plant producing the herbicide, exposed workers complained of nausea, headache, fatigue and muscular aches and pains (31).

No causal association could be found between the long-time exposure of workers engaged in the manufacture of the compounds and their mortality rates from malignant neoplasms (cancers of the stomach, liver, connective tissue, lymphomas, and nasopharyngeal system). A statistically significant association was obtained between exposure and mortality from cirrhosis of the liver, but this could be due to alcohol abuse (32).

Cohort mortality studies on forestry workers exposed to phenoxyacid herbicides such as 2,4,5-T showed a statistically significant excess number of deaths due to suicide (33).

Birth malformations in the Northland region of New Zealand, where the compound was sprayed aerially ~1 × month⁻¹ from 1960-1977, were studied. Heart malformations, hypospadias and epispadias increased with spraying density, but the increases were not statistically significant. The incidence of club foot (talipes) did increase in a statistically significant manner. No association was found with central nervous system defects, nor with cleft lip or palate (34).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (35).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (36).

Tolerable daily intake (TDI) humans 0.03 mg kg⁻¹ (12).

Other comments

Residues have been detected in ground water (1).

In Europe, residues of 0.05 mg kg⁻¹ have been found on grain and 1 mg kg⁻¹ on the straw of wheat, barley, oats and rye (12).

Technical 2,4,5-T contains traces of the highly toxic compound 2,3,7,8-tetrachlorodibenzo-*p*-dioxin which can cause chloracne in exposed workers (1).

In March 1985, the US EPA stopped all registrations for the use of this herbicide. This follows the 1970 action of the Department of Agriculture (37).

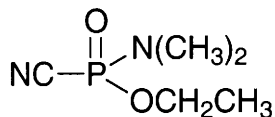
Human health hazards, experimental toxicology reviewed (38,39).

Agent Orange, a mixture of the butyl esters of 2,4-D and 2,4,5-T was used extensively during the US intervention in Vietnam, for defoliation.

References

1. *Drinking Water Health Advisory: Pesticides* 1989, Lewis Publishers, Chelsea, MI, USA.
2. *The Pesticide Manual* 9th ed., 1991, British Crop Protection Council, Farnham, UK.
3. Rehwoldt, R. E. et al *Bull. Environ. Contam. Toxicol.* 1977, **18**, 361-365.
4. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 316-431.
5. Kenaga, E. E. *Down to Earth* 1979, **35**(2), 25-31.
6. Walsh, G. E. *Hyacinth Control J.* 1972, **10**, 45-48.
7. Yockim, R. S. et al *Chemosphere* 1978, **7**, 215.
8. Garcia, J. D. et al *Bull. Environ. Contam. Toxicol.* 1979, **23**, 231-235.
9. Gibson, S. A. et al *Appl. Environ. Microbiol.* 1990, **56**(6), 1825-1832.
10. Alexander, M. *Microbiol. Degradation of Pesticides in Environmental Toxicology of Pesticides* 1972, Matsumura, F. (Ed.) Academic Press, New York, NY, USA.
11. Edwards, C. A. *Residue Rev.* 1966, **13**, 83.
12. *WHO/Food Add./71.42* 1971, 459-477.
13. *Fundam. Appl. Toxicol.* 1986, **7**, 299.
14. Drill, V. A. et al *Arch. Ind. Hyg. Occup. Med.* 1953, **7**, 61-67.
15. Vos, J. G. et al *Pestic. Chem. Hum. Welfare Environ., Proc. 5th Int. Congr. Pestic. Chem.* 1983, **3**, 497-504.
16. *IARC Monograph* 1987, **Suppl. 7**, 60.
17. Kociba, R. J. et al *Food Cosmet. Toxicol.* 1979, **17**, 205-221.
18. Seidenberg, J. M. et al *Teratog., Carcinog., Mutagen.* 1987, **7**(1), 17-28.
19. Dougherty, W. J. et al *Environ. Qual. Saf.* 1976, **5**, 89-96.
20. Emerson, J. L. et al *Food Cosmet. Toxicol.* 1971, **9**, 395-404.
21. Roll, R. *Food Cosmet. Toxicol.* 1971, **9**(5), 671-676.
22. Grunow, W. et al *Food Cosmet. Toxicol.* 1971, **9**, 667-670.
23. Gehring, P. J. et al *Toxicol. Appl. Pharmacol.* 1973, **25**(3), 441.
24. Fang, S. C. et al *Toxicol. Appl. Pharmacol.* 1973, **24**(4), 555-563.
25. Gehring, P. J. et al *Ecol. Bull.* 1978, **27**, 122-133.
26. Soler-Niedziela, L. et al *Toxic. Assess.* 1988, **37**(2), 137-145.
27. Mersch-Sundermann, V. et al *Zentralbl. Hyg. Umweltmed.* 1989, **189**(2), 135-146 (Ger.) (*Chem. Abstr.* **112**, 113966u).
28. Galloway, S. M. et al *Environ. Mol. Mutagen.* 1987, **10**(Suppl. 10), 1-175.
29. Shirasu, Y. et al *Mutat. Res.* 1967, **40**, 19-30.
30. Jenssen, D. et al *Chem. Biol. Interact.* 1976, **14**(3-4), 291-299.
31. Zack, J. A. et al *J. Occup. Med.* 1980, **22**(1), 1-14.
32. Ott, M. G. et al *J. Occup. Med.* 1987, **29**(5), 422-429.
33. Green, L. M. *Scand. J. Work, Environ. Health* 1987, **13**(5), 460.
34. Hanify, J. A. et al *Science* 1981, **212**(4492), 349-351.
35. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
36. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
37. *Chem. Eng. News* 1985, **63**(6).
38. *Report* 1989, EPA/600/8-88/058, Order No. PB90-142365, Available from NTIS.
39. *IARC Monograph* 1986, **41**, 357-406

T2 Tabun



$C_5H_{11}N_2O_2P$

Mol. Wt. 162.13

CAS Registry No. 77-81-6

Synonyms dimethylphosphoramidocyanidic acid, ethyl ester; ethyl *N*-dimethylphosphoramidocyanidate; GA

RTECS No. TB 4550000

Uses Military nerve gas.

Physical properties

M. Pt. $-50^{\circ}C$ B. Pt. $240^{\circ}C$ Flash point $78^{\circ}C$ Specific gravity 1.077 Volatility v.p. 0.07 mmHg at $25^{\circ}C$; v.den. 5.63

Solubility Water: miscible, but rapidly hydrolysed. Organic solvents: soluble in most organic solvents

Mammalian & avian toxicity

Acute data

LD₅₀ oral dog 200 $\mu g\ kg^{-1}$ (1).

LD₅₀ dermal monkey 9300 $\mu g\ kg^{-1}$ (2).

LC₅₀ (10 min) inhalation monkey 250 $mg\ m^{-3}$ (2).

LD₅₀ subcutaneous rat 193 $\mu g\ kg^{-1}$ (3).

LD₅₀ intravenous for inhibition of acetylcholinesterase in whole mouse brain was 0.287 $mg\ kg^{-1}$. The ED₅₀ was 69% of the LD₅₀ (4).

Genotoxicity

In vitro Chinese hamster ovary cells 200 $\mu g\ ml^{-1}$ with and without metabolic activation positive. Sister chromatid exchange increased linearly with increased concentration (5).

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with metabolic activation weakly positive, without metabolic activation negative (6).

In vitro mouse lymphoma cell L5178Y with and without metabolic activation positive (7).

Other effects

Other adverse effects (human)

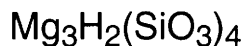
Potent inhibitor of cholinesterase activity. This inhibition results in both muscarinic and nicotinic effects with some central involvement. Signs of toxicity include abdominal cramps, nausea, vomiting, diarrhoea, urinary incontinence, eye changes, weakness, respiratory disturbances, lachrymation, increased salivation and sweating, bradycardia or tachycardia, hypotension or hypertension, cyanosis, muscular twitching and convulsions. May cause delayed neuropathy. Central nervous symptoms include restlessness, anxiety, dizziness, confusion, coma, and depression of the respiratory or cardiovascular system. Mental disturbance may be experienced (8).

References

1. *Deutsches Gesundheitswesen* 1960, **15**, 2179.
2. *National Technical Information Service* PB158-508, Springfield, VA, USA.
3. *Archives International de Pharmacodynamic et de Therapie* 1983, **262**, 231.
4. Tripathi, H. L. et al *J. Toxicol. Environ. Health* 1989, **26**(4), 437-446.
5. Nasr, M. et al *Gov. Rep. Announce. Index. (U.S.)* 1990, **90**(6), Abstr. No. 012,522.

6. Goldman, M. et al *Gov. Rep. Announce. Index. (U.S)* 1990, **90**(23), Abstr. No. 61,240.
7. Kawakami, T. G. et al *Gov. Rep. Announce. Index (U.S.)* 1990, **90**(4), Abstr. No. 008,176.
8. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK

T3 talc



$\text{H}_2\text{Mg}_3\text{O}_{12}\text{Si}_4$

Mol. Wt. 379.27

CAS Registry No. 14807-96-6

Synonyms Talcum; French chalk; Soapstone; Steatite; Lubestine

EINECS No. 238-877-9

RTECS No. WW 2710000

Uses Dusting powder for medicinal and toilet preparations. Excipient for pills and tablets. Pigment in paints, varnishes and rubber.

Occurrence Talc rocks. Finely powdered native hydrous magnesium silicate.

Physical properties

Specific gravity 2.58-2.83

Occupational exposure

DE-MAK 2 mg m⁻³ (without asbestos fibres) (respirable fraction of aerosol)

SE-LEVL 2 mg m⁻³ (total dust); 1 mg m⁻³ (respirable dust)

UK-LTEL 1 mg m⁻³ (respirable dust)

US-TWA 2 mg m⁻³ (respirable fraction containing no asbestos fibres and <1% crystalline silica)

Mammalian & avian toxicity

Acute data

3/11 rats died within 24 hr following injections of 1400 mg kg⁻¹ into the lower pole of the spleen (1).

Sub-acute and sub-chronic data

Intravenous (2 wk) rabbit 100 mg day⁻¹, mild to marked arterial endothelial cell proliferation with cellular encroachment into the lumen and the occurrence of foreign-body giant cells within the endothelial masses were observed (2).

Intratracheal (duration unspecified) chinchillas 40 mg in saline, chronic pulmonary irritation and proliferative pneumonia, with giant-cell granulomas and adjacent metaplasia of the alveolar epithelium were observed (3).

Inhalation (3 month) rat 10.8 mg m⁻³ minimal fibrosis was observed, the degree of which did not change during the post-exposure period (4).

Carcinogenicity and chronic effects

Intraperitoneal (86 wk) 40 ♀ Wistar rats, four injections of 5 mg in 2 ml saline at wkly intervals. A mesothelioma was observed in 1/36 exposed rats and none in 72 controls (5).

Subcutaneous (85 wk) 50 ♀ R3 mice were given 0.2 ml of a mixture of 8 g talc and 20 g peanut oil. No local tumours were observed (6).

Intrapleural (2 yr) 24 ♂ and ♀ Wistar rats 20 mg Italian talc. No mesothelioma was detected in either group, one small pulmonary adenoma was found in one rat that died 25 months after injection (4).

Teratogenicity and reproductive effects

Talc was found to produce nonspecific abnormalities in chicken eggs, at an incidence similar to that induced by thalidomide (7).

Oral rats, mice 1600 mg kg⁻¹ on days 6-15 of gestation; hamsters 1200 mg kg⁻¹ on days 6-10 of gestation; rabbits 900 mg kg⁻¹ on days 6-18 of gestation. No teratological effects were observed (8).

Metabolism and toxicokinetics

Inhalation (4 wk) 20 F344/Crl rats and 20 B6C3F₁ mice, 0, 2.3, 4.3, 17 mg m⁻³ and 0, 2.2, 5.7 and 20.4 mg m⁻³, respectively, for 6 hr day⁻¹, 5 day wk⁻¹. Lung burdens in rats averaged 0, 0.97, 0.17 and 0.72 mg g⁻¹ lung, respectively after the 20-day inhalation exposure, in mice 0, 0.10, 0.29 and 1.0 mg g⁻¹ lung respectively (9). Inhalation rat 10.8 m⁻³, the mean amounts retained in the lungs were 2.5, 4.7 and 12.2 mg rat⁻¹ following exposure for 3, 6 and 12 months, respectively (4). Inhalation rat 2.3, 4.3 and 17 mg m⁻³ 6 hr day⁻¹, 5 day wk⁻¹ for 4 wk. Amounts retained in the lung at the end of exposure were 77, 187 and 806 µg g⁻¹ lung, respectively (10).

Genotoxicity

Salmonella typhimurium TA1530, G46 (metabolic activation unspecified) negative (11).

Saccharomyces cerevisiae D3 (metabolic activation unspecified) negative (11).

Rat pleural mesothelial cell genotoxicity assays (unscheduled DNA synthesis and sister chromatid exchanges) negative using talc consisting of particles of respirable size (12).

Oral rat 30-5000 mg kg⁻¹ neither chromosomal aberrations nor dominant lethal mutations were induced (11).

In vitro human W138 cells 2-200 µg ml⁻¹ chromosomal aberrations were not induced (11).

Other effects

Other adverse effects (human)

Talc particles, but no other insoluble particles, were found in the subserosal stroma of hernia sacs in humans, possibly due to ingestion of medications containing talc as a filler (13).

Contamination of wound or body cavities with talc is liable to cause granulomas. Prolonged or intense aspiration of talc may produce pneumoconiosis (14).

A variety of pathological effects arise from intravenous use of talc-containing drugs for addicts. These include pulmonary opacities, angiothrombotic pulmonary hypertension, conglomerate pulmonary lesions, retinopathy, cerebral microembolisation and granulomas of the liver, lymph nodes and kidneys (15-17). Of 176 talc workers, 27% suffered from pneumoconiosis, which was highly related to dust exposure levels (18).

In vitro 65 mg ml⁻¹ caused 50% haemolysis of red blood cells (19).

Other comments

Inhalation toxicity to the lungs reviewed (20,21).

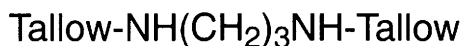
Cosmetic uses of talc reviewed (22).

References

1. Egar, W. et al *Beitr. Silikose-Forsch.* 1964, **81**, 12-42.
2. Puro, H. E. et al *J. Am. Med. Assoc.* 1966, **197**, 1100-1102.
3. Trautwein, G. et al *Pathol. Vet.* 1967, **4**, 254-267.
4. Wagner, J. C. et al *Inhaled Particles* 1977, **IV**(2), 647-654, Pergamon Press, Oxford, UK.
5. Pott, F. et al *Environ. Health Perspect.* 1974, **9**, 313-315.
6. Neukomm, S. et al *Med. Exp.* 1961, **4**, 298-306.
7. Carter, S. B. *Advances in Toxicological Methodology* 1965, **V**, 142-149, Elsevier, Amsterdam, Netherlands.
8. Food and Drug Research Laboratories *Teratologic Evaluation of FDA 71-43 (TALC)* 1973, National Technical Information Service, Washington, DC, USA.
9. Pickrell, J. A. et al *Environ. Res.* 1989, **49**(2), 233-245.
10. Hanson, R. L. et al *J. Appl. Toxicol.* 1985, **5**, 283-287.
11. Liton Bionetics *Mutagenic Evaluation of Compound FDA-71-43; (TALC CPB245458)* 1974, National Technical Information Service.
12. Endo-Capron, S. et al *Toxicol. In Vitro* 1993, **7**(1), 7-14.
13. Pratt, P. C. et al *Human Pathol.* 1985, 1141-1146.

14. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
15. Tao, L.-C. et al *Acta Cytol.* 1984, **28**, 737-739.
16. Crouch, E. et al *Am. J. Clin. Pathol.* 1983, **80**, 520-526.
17. Carman, C. R. *J. Am. Optom. Assoc.* 1985, **56**, 129-130.
18. Leophonte, P. et al *NATO ASI Ser., Ser. G* 1990, **21**(Health Relat. Eff. Phyllosilicates), 203-209.
19. Woodworth, C. D. et al *Environ. Pathol.* 1982, **27**, 190-205.
20. Wagner, J. C. *NATO ASI Ser., Ser. G* 1990, **21**(Health Relat. Eff. Phyllosilicates).
21. Mannfred, A. *Toxicol. Lett.* 1990, **52**(2), 121-127.
22. Grexa, R. W. et al *Drug. Cosmet. Ind.* 1987, **140**(5), 56-60

T4 **N-tallow-1,3-propanediamine**



CAS Registry No. 61791-55-7

Synonyms N-alkyl-1,3-propanediamine

EINECS No. 263-189-0

Uses In water treatment (1).

Ecotoxicity

Invertebrate toxicity

LC₅₀ larvae and pupae Southern house mosquito 0.9 mg kg⁻¹ (2,3).

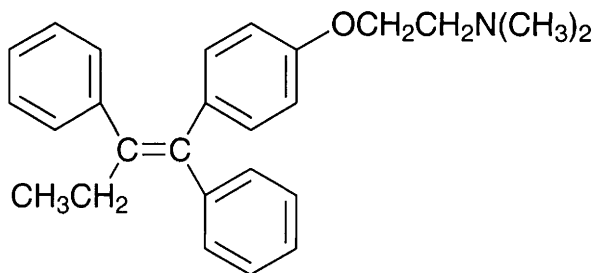
Other comments

When a series of long-chain aliphatic diamines of the general formation RR₁N(CH₂)_nNR₂C₂H_{2n+1} were tested *in vitro* for their activity against *Streptococcus mutans*, all compounds with n=14-18 showed high activity (4).

References

1. Moran, F. *Fr. Demande* No 2359076, 17 Feb 1978 (*Chem. Abstr.* **90**, 141902r).
2. Mulla, M. S. et al *J. Econ. Entomol.* 1970, **63**, 1972.
3. Mulla, M. S. et al *J. Econ. Entomol.* 1970, **60**, 115.
4. Bass, G. E. et al *J. Dent. Res.* 1975, **54**, 972

T5 tamoxifen



C₂₆H₂₉NO

Mol. Wt. 371.52

CAS Registry No. 10540-29-1

Synonyms [Z]-2-[4-(1,2-diphenyl-1-butenyl)-phenoxy]-N,N-dimethylethanamine; 1-*p*-β-dimethylaminoethoxyphenyl-*trans*-1,2-diphenylbut-1-ene; Nolvadex

EINECS No. 234-118-0

RTECS No. KR 5919500

Uses Oestrogen antagonist. Inhibits the production or release of cellular growth factors. Used (as the citrate) in the adjuvant endocrine therapy of early breast cancer and in the palliative treatment of the advanced disease. Used to stimulate ovulation in women with anovulatory infertility (1).

Physical properties

M. Pt. 96-98°C

Solubility Water: slightly soluble. Organic solvents: methanol, very slightly soluble in acetone and in chloroform

Environmental fate

Degradation studies

In screening studies of tamoxifen bioconversion by microbes, only *Streptomyces rimosus* ATCC 2234 metabolised the compound to 4-hydroxytamoxifen. A number of microorganisms transformed tamoxifen to tamoxifen-*N*-oxide and desmethyltamoxifen (2).

Only 1 of 96 fungi examined transformed tamoxifen. *Gliocladium roseum* transformed the compound to *N*-desmethyltamoxifen and tamoxifen-*N*-oxide (3).

Mammalian & avian toxicity

Carcinogenicity and chronic effects

Alderley Park Wistar-derived rats (2 yr) 5, 20, or 35 mg kg⁻¹ tamoxifen daily by gastric intubation. A dose-related increase in the incidence of hepatocellular tumours occurred, which was first observed after 31 wk treatment in the top dose group (4).

Teratogenicity and reproductive effects

Genital tracts isolated from 4-19 wk-old human ♀ foetuses were grown for 1-2 months in untreated athymic nude mice, or host mice treated by subcutaneous pellet with tamoxifen. Oestrogenic and potentially teratogenic effects on the developing human genital tract were observed (5).

Metabolism and toxicokinetics

Following an oral dose in humans, plasma concentrations of tamoxifen occur after 4-7 hr. Plasma clearance is biphasic; terminal *t*_{1/2} may be >7 days. Extensively metabolised, with the major metabolite being *N*-desmethyltamoxifen. Excreted slowly in faeces, mainly as conjugates. Undergoes enterohepatic circulation (1). Experimental evidence has been obtained that the metabolic activation of tamoxifen to species that form adducts with DNA leading to hepatocarcinoma in mice, rats, and hamsters involves α-hydroxylation of the ethyl group (6). Tamoxifen is metabolically activated in ICR mice to DNA-reactive compounds along two distinct pathways, one sensitive to and the other resistant to the sulfotransferase inhibitor pentachlorophenol (7).

Genotoxicity

Not genotoxic in conventional genotoxicity studies (4).

Other effects

Other adverse effects (human)

Tamoxifen is generally well-tolerated in patients, with the most frequent adverse effects being hot flushes, nausea and vomiting. Other adverse effects include oedema, vaginal bleeding or discharge, pruritus vulvae, rashes, and dry skin (1).

Side-effects of long-term treatment with tamoxifen are few and generally mild. The serious effects, except eye toxicity, appear to be due to its mild oestrogen-like action (8).

Tamoxifen treatment increases the risk of endometrial cancer in women. The formation of DNA adducts in leucocytes and endometrial samples from tamoxifen-treated women suggests that it may be genotoxic to humans (9).

Any other adverse effects

It has been shown that tamoxifen exhibits both oestrogenic and anti-oestrogenic activities in roosters from investigations of its modulation of the hepatic expression of oestrogen-regulated mRNA stabilising factor (10).

Other comments

DNA adducts with tamoxifen reviewed (11).

The mycoestrogen α -zearalanol induced acute hepatotoxicity and, subsequently, hepatic carcinogenesis in the Armenian hamster. Both effects were blocked by tamoxifen, which suggests oestrogen receptor mediation (12).

Carcinogenicity in humans reviewed. Data from randomised trials indicates that there is a small, but real, increased risk of endometrial cancer in women taking tamoxifen (13).

References

1. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
2. El-Sharkawy, S. H. *Pharm. Acta Helv.* 1992, **67**(1), 15-19.
3. El-Sharkawy, S. et al *Pharm. Res.* 1987, **4**(4), 353-354.
4. Greaves, P. et al *Cancer Res.* 1993, **53**(17), 3919-3924.
5. Cunha, G. R. et al *Hum. Pathol.* 1987, **18**(11), 1132-1143.
6. Phillips, D. H. et al *Carcinogenesis* 1994, **15**(8), 1487-1492.
7. Randerath, K. et al *Carcinogenesis* 1994, **15**(5), 797-800.
8. Cobelli, S. et al *J. Chemother. (Florence)* 1997, **9**(4), 300-303.
9. Marques, M. M. et al *Carcinogenesis* 1997, **18**(10), 1949-1954.
10. Ratnasabapathy, R. et al *Biochem. Pharmacol.* 1997, **53**(10), 1425-1434.
11. Busch, H. *Semin. Oncol.* 1997, **24**(1, Suppl. 1), S98-S104.
12. Coe, J. E. *Proc. Natl. Acad. Sci. U.S.A.* 1992, **89**(3), 1085-1089.
13. Stearns, V. et al *J. Clin. Oncol.* 1998, **16**, 779-792.

T6 tannic acid

$C_{76}H_{52}O_{46}$

Mol. Wt. 1701.22

CAS Registry No. 1401-55-4

Synonyms gallotannic acid; tannin; glycerite

EINECS No. 215-753-2

RTECS No. WW 5075000

Uses Tanning, mordant in textile dyeing, clarification agent in wine manufacture, photography, alcohol denaturant. Also as an astringent for the mucous membranes of the mouth and throat and in suppositories for the treatment of haemorrhoids. Formerly added to barium sulfate enemas.

Occurrence Natural and widely occurring astringent or tanning agent found in tree barks, nutgalls and other plant parts.

Physical properties

B. Pt. 200°C Flash point 199°C (open cup)

Solubility Water: 2857 g l⁻¹. Organic solvents: acetone, ethanol

Ecotoxicity

Fish toxicity

Toxic to goldfish at 100 ppm (1).

Environmental fate

Nitrification inhibition

10-25% inhibition of NH₃ oxidation by *Nitrosomonas* sp. at 100 mg l⁻¹; 7% inhibition at 50 mg l⁻¹ (2).

Degradation studies

BOD₅ 0.31; standard dilution technique with normal sewage as seed material 0.46 (3,4).

Mammalian & avian toxicity

Acute data

LD₅₀ gavage redwinged blackbird >100 mg kg⁻¹ (5).

LD_{Lo} oral mouse 2000 mg kg⁻¹ (6).

LD_{Lo} intravenous mouse 10 mg kg⁻¹ (6).

LD₅₀ oral mouse 3500 mg kg⁻¹ (6).

LD_{Lo} subcutaneous mouse 75 mg kg⁻¹ (6).

LD₅₀ intravenous mouse 40 mg kg⁻¹ (6).

LD₅₀ intramuscular mouse 350 mg kg⁻¹ (7).

LD_{Lo} oral rat 200 mg kg⁻¹ (8).

LD₅₀ subcutaneous rat 1500 mg kg⁻¹ (9).

LD_{Lo} parenteral rat 1400 mg kg⁻¹ (10).

LD₅₀ oral rat 2260 mg kg⁻¹ (11).

LD₅₀ oral rabbit 5000 mg kg⁻¹ (12).

Subcutaneous rat 250 mg kg⁻¹ resulted in centrilobular necrosis of the liver (13).

Carcinogenicity and chronic effects

No adequate data for carcinogenicity to humans, limited evidence for carcinogenicity to animals, IARC classification group 3 (14,15).

Subcutaneous mice (12 wk) 0.25 ml weekly. After one year it was seen that condensed tannins caused local sarcomas and liver tumours, but hydrolysable tannins only liver tumours (15).

Subcutaneous ♂ and ♀ rats (290 days) aqueous tannic acid every fifth day (initial dose 150 mg kg⁻¹ body weight, then 200 mg kg⁻¹) suffered liver tumours (15).

Teratogenicity and reproductive effects

Laying hens (8 wks) fed 1-2% tannic acid in corn-soybean meal basal diet marginal in methionine (0.25%) and choline (831 mg kg⁻¹) suffered decrease in body weight, egg weight and production, and increased egg yolk mottling. High tannin (1.20 or 1.24%) grain sorghums had no significant effect on egg production, egg weight, or yolk mottling, but did significantly reduce body weight when added at 50% to the basal diet for 4 wk (16).

Metabolism and toxicokinetics

Absorption of tannic acid from the colon has been demonstrated in rabbits, sheep, goats, rats and dogs (17,18). Tannic acid injected intraperitoneally or subcutaneously into rats was detected in the liver after one hour, and in the nuclei after three hours. The sequence of events leading to liver damage was: concentration of tannic acid in nuclei, inhibition of nuclear RNA synthesis, inhibition of protein synthesis and production of necrosis (13,19,20).

Other effects

Other adverse effects (human)

The use of tannic acid-containing barium enemas has been suggested to be associated with eight deaths due to acute liver failure (18,21).

In unskilled hands, its application to produce partial thickness burns in tattoo removal has resulted in full thickness burns requiring skin grafting (22).

Other comments

Carcinogenic risks to humans reviewed (15).

References

1. Grindley, *Ann. Appl. Biol.* 1946, **33**, 103.
2. Hockenbury, M. R. et al *J. Water Pollut. Control Fed.* 1977, **49**(5), 768-777.
3. Meissner, B. *Wasserwirtsch.-Wassertech.* 1954, **4**, 166.
4. Weston, R. S. *Activated Carbon in Sewage and Industrial Waste Treatment*, Masters Thesis, New York University, 1939.
5. Schafer, E. W., Jr. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
6. Robinson, H. J. et al *Pharmacol. Exp. Ther.* 1943, **77**, 63-69.
7. Armstrong, D. M. G. et al *J. Pharm. Pharmacol.* 1957, **9**, 98-101.
8. *Wien. Klin. Wochenschr.* 1950, **62**, 270.
9. Cameron, G. R. et al *Lancet* 1943, **ii**, 179-186.
10. *Food Cosmet. Toxicol.* 1976, **14**, 565.
11. Boyd, E. M. *Can. Med. Assoc. J.* 1965, **92**, 1292-1297.
12. *Am. J. Vet. Res.* 1962, **23**, 1264.
13. Horvath, E. et al *Brit. J. Exp. Pathol.* 1960, **41**, 298-304.
14. *IARC Monograph* 1987, **Suppl. 7**, 72.
15. *IARC Monograph* 1976, **10**, 253-262.
16. Armanious, M. W. et al *Poult. Sci.* 1973, **52**(6), 2160-2168.
17. Dollahite, J. W. et al *Am. J. Vet. Res.* 1962, **23**, 1264-1267.
18. McAlister, W. H. et al *Radiology* 1963, **80**, 765-773.
19. Badawy, A. A. B. et al *Biochem. J.* 1969, **113**, 307-313.
20. Reddy, J. K. et al *Cancer Res.* 1970, **30**, 58-65.
21. Lucke, H. H. et al *Can. Med. Assoc. J.* 1963, **89**, 1111-1114.
22. Scott, M. et al *Br. Med. J.* 1991, **303**, 720

T7 tantalum

Ta

Ta

Mol. Wt. 180.95

CAS Registry No. 7440-25-7

EINECS No. 231-135-5

RTECS No. WW 5505000

Uses In pen points. Analytical weights. Apparatus and instruments for chemical, dental and surgical use instead of platinum.

Occurrence As tantalite, columbite, euxenite and microlite. Almost always associated with niobium.

Physical properties

M. Pt. 2996°C B. Pt. 5429°C Specific gravity 16.69

Occupational exposure

DE-MAK 4 mg m⁻³ (inhalable fraction of aerosol)

FR-VME 5 mg m⁻³

UK-LTEL 5 mg m⁻³

UK-STEL 10 mg m⁻³

US-TWA 5 mg m⁻³ (dust)

Ecotoxicity

Bioaccumulation

It was detected in the marine phanerogam *Posidonia oceanica* (1).

Mammalian & avian toxicity

Acute data

Oral rat 8000 mg kg⁻¹ nontoxic (form of tantalum unspecified) (2).

Carcinogenicity and chronic effects

50 implants of tantalum metal in 25 Wistar rats (2 yr) induced 2 malignant fibrosarcomas (3).

Metabolism and toxicokinetics

In young and adult rats the amount of tantalum nuclide absorbed following oral administration was several orders of magnitude greater in young suckling rats than in adults, with an initial rapid loss of the nuclide by weaning time (3 wk). Distribution of ¹⁸²Ta was greatest in the ileum, kidney and bone (4).

In studies on rabbits it was found that intramedullary nails of tantalum are not inert in the body and that its corrosion products undergo transport processes (5).

A study using ¹⁸²Ta showed that tantalum has a high affinity for proteins in humans (6).

Other effects

Other adverse effects (human)

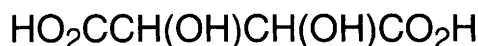
Three reactor workers accidentally inhaled tantalum oxide. The whole body retention after 7 days was 1% of the initial deposit. In one subject studied for a further 424 days, the residual activity in the thorax was cleared with a biological t_{1/2} of 1400 days. Tantalum powder administered by inhalation has prolonged alveolar retention (7).

Administered acutely and chronically, it is nontoxic by all routes and concentrations encountered under industrial conditions (2).

References

1. Augier, H. et al *Mar. Biol. (Berlin)* 1991, **109**(2), 345-353.
2. *Patty's Industrial Hygiene and Toxicology* 3rd rev. ed., 1981, John Wiley & Sons, New York, NY, USA.
3. Oppenheimer, B. S. et al *Cancer Res.* 1956, **16**, 456.
4. Shiraishi, Y. et al *J. Radiat. Res. (Tokyo)* 1972, **13**, 14.
5. Michel, R. et al *Trace Elem. Anal. Chem. Med. Biol. Proc. Int. Workshop*, 5th 1988, 504-512.
6. Edel, J. et al *Sci. Total. Environ.* 1990, **95**, 107-117.
7. Newton, D. *Am. J. Roentgenol.* 1977, **32**, 129

T8 DL-tartaric acid



$\text{C}_4\text{H}_6\text{O}_6$

Mol. Wt. 150.09

CAS Registry No. 133-37-9

Synonyms 2,3-dihydroxybutanedioic acid; uvic acid; racemic tartaric acid

EINECS No. 205-105-7

Physical properties

M. Pt. 206°C Specific gravity 1.697 Partition coefficient $\log P_{\text{ow}} -0.76$ (1)

Solubility Water: 20.6 g l⁻¹ at 20°C. Organic solvents: diethyl ether, ethanol

Ecotoxicity

Fish toxicity

Trout perturbation level 150 mg l⁻¹ (duration unspecified) (1).

LC₅₀ goldfish, lifetime exposure in hard water 200 mg l⁻¹ lifetime exposure in very soft water 10 mg l⁻¹ (duration unspecified) (2).

Invertebrate toxicity

Vorticella campanula perturbation level 100 mg l⁻¹ (duration unspecified) (1).

LC₀ *Paramecium caudatum* 250-320 mg l⁻¹ (duration unspecified) (1).

Gammarus pulex perturbation level 230 mg l⁻¹ (duration unspecified) (1).

Environmental fate

Degradation studies

BOD₅ 0.350 mg O₂ l⁻¹ (1).

Wastewater treatment activated sludge, 2.6% ThOD after 6 hr; 1.4% of ThOD after 12 hr and 0.7% of ThOD after 24 hr (1).

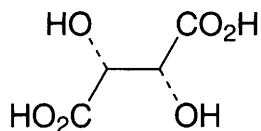
Other comments

It has an inhibitory effect on calcium oxalate urolithiasis (3).

References

1. Meinck, F. et al *Les Eaux Residuaries Industrielles* 1970.
2. Ellis, M. M. *U.S. Bur. Fisheries Bull.* 1937, No. 22, XLVIII, 365-437, U.S. Dept. Commerce, Washington, DC, USA.
3. Selvam, G. S. et al *Med. Sci. Res.* 1990, **18**(8), 313-315

T9 L-tartaric acid



$C_4H_6O_6$

Mol. Wt. 150.09

CAS Registry No. 87-69-4

Synonyms [R-(R*,R*)]-2,3-dihydroxybutanedioic acid; natural tartaric acid; *d*- α,β -dihydroxysuccinic acid

EINECS No. 201-766-0

RTECS No. WW 7875000

Uses In soft drink industry. Confectionery products. In photography. Pharmaceutic aid buffering agent.

Occurrence Widely distributed in nature, classified as a fruit acid.

Physical properties

M. Pt. 168-170°C **Specific gravity** 1.7598 at 20°C with respect to water at 4°C

Solubility Water: 115 g l⁻¹ at 0°C, 156 g l⁻¹ at 30°C. Organic solvents: diethyl ether, ethanol, methanol, propanol

Mammalian & avian toxicity

Acute data

LD_{Lo} oral dog, rabbit 5000 mg kg⁻¹ (1,2).

LD₅₀ intravenous mouse 485 mg kg⁻¹ (3).

Metabolism and toxicokinetics

Absorbed from the gastro-intestinal tract (species unspecified), but up to 80% of an ingested dose is probably destroyed by microorganisms in the lumen of the intestine before absorption occurs. Absorbed tartaric acid is excreted in the urine unchanged (4).

Other effects

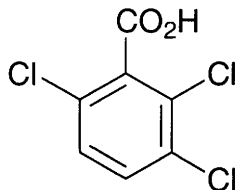
Other adverse effects (human)

Strong solutions of tartaric acid are mild irritants and if ingested undiluted may cause gastro-enteritis (4).

References

1. *J. Agric. Food Chem.* 1957, **5**, 759.
2. *J. Am. Pharm. Assoc., Scientific Edition* 1950, **39**, 275.
3. *Ind. Eng. Chem.* 1923, **15**, 628.
4. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK

T10 2,3,6-TBA



$C_7H_3Cl_3O_2$

Mol. Wt. 225.46

CAS Registry No. 50-31-7

Synonyms 2,3,6-trichlorobenzoic acid; Benzabar; Benzac; Fen-All; 2,3,6-TCB; 2,3,6-TCBA; Tribac; Triben; Zobar

EINECS No. 200-026-4

RTECS No. DH 7700000

Uses Herbicide.

Physical properties

M. Pt. 124-126°C; 87-99°C (technical grade) **Volatility** v.p. 2.4×10^{-2} mmHg at 100°C

Solubility Water: 7.7 g l⁻¹ at 22°C. Organic solvents: acetone, benzene, chloroform, diethyl ether, ethanol, xylene

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed (R22)

Safety phrases Keep out of reach of children (if sold to general public) – Do not breathe dust (S2, S22)

Environmental fate

Degradation studies

Supported the growth of *Pseudomonas putida* P111 (1).

30-50% dechlorination by microorganisms in soil after 1-5 months (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral chicken >1500 mg kg⁻¹ (3).

LD₅₀ oral rat, mouse, rabbit, guinea pig 610-1500 mg kg⁻¹ (4,3).

LD₅₀ subcutaneous mouse 1500 mg kg⁻¹ (5).

LD₅₀ intraperitoneal mouse, rat 180, 1000 mg kg⁻¹, respectively (6,7).

Sub-acute and sub-chronic data

Oral rat (69 day) 1000 or 10,000 mg kg⁻¹ diet; the high dose caused a minor disturbance of water metabolism (3).

Metabolism and toxicokinetics

Largely excreted unchanged in the urine following oral administration to rats (3).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (8).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (9).

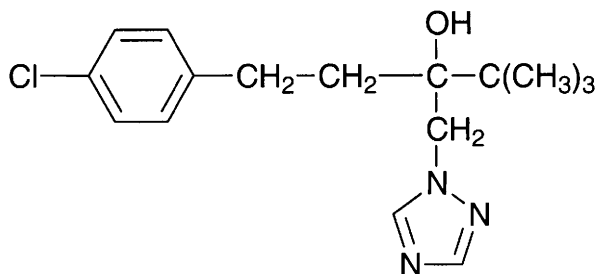
Other comments

Metabolic pathways reviewed (10).

References

1. Hernandez, B. S. et al *Appl. Environ. Microbiol.* 1991, **57**(1), 3361-3366.
2. Dewey, O. R. et al *Nature* 1962, **195**, 1232.
3. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
4. *Hyg. Sanit.* 1970, **35**(7-9), 14.
5. *Biochem. Pharmacol.* 1964, **13**, 1538.
6. *J. Med. Chem.* 1968, **11**, 1020.
7. *Guide To Chemicals Used in Crop Protection* 1973, **6**, 515.
8. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
9. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
10. Roberts, T. R. et al (Eds.) *Metabolic Pathways of Agrochemicals. Part 1: Herbicides and Plant Growth Regulators* 1998, The Royal Society of Chemistry, Cambridge, UK

T11 tebuconazole



C₁₆H₂₂ClN₃O

Mol. Wt. 307.82

CAS Registry No. 107534-96-3

Synonyms (RS)-1-(4-chlorophenyl)-4,4-dimethyl-3-((1H-1,2,4-triazol-1-ylmethyl)pentan-3-ol);
(±)-α-[2-(4-chlorophenyl)ethyl]-α-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol

EINECS No. 403-640-2

RTECS No. XZ 4803270

Uses Fungicide which inhibits ergosterol biosynthesis.

Physical properties

M. Pt. 102.4°C **Specific gravity** 1.25 at 26°C **Partition coefficient** log P_{ow} 3.7 (1)

Volatility v.p. 1.3 μPa at 20°C

Solubility Water: 32 mg l⁻¹ at 20°C. Organic solvents: dichloromethane, hexane, isopropanol, toluene

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) rainbow trout, golden orfe 6.4, 8.7 mg l⁻¹, respectively (1).

Invertebrate toxicity

EC₅₀ (48 hr) *Daphnia* 10-12 mg l⁻¹ (1).

Non-toxic to bees (1).

Environmental fate

Degradation studies

Degradation in soil was slow in laboratory studies, but under field conditions the compound degraded much more rapidly (1).

Abiotic removal

Volatilisation trials were carried out with tebuconazole using appropriate target crops and at application times to ensure typical weather conditions. The compound shows <20% volatilisation (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral ♂ Japanese quail, ♀ Japanese quail, bobwhite quail 4438, 2912, 1988 mg kg⁻¹, respectively (1).

LD₅₀ oral rat 4000 mg kg⁻¹ (1).

LD₅₀ oral mouse 3000 mg kg⁻¹ (1).

LC₅₀ (4 hr) inhalation rat >0.8 mg l⁻¹ (aerosol), >5.1 mg l⁻¹ (dust) (1).

LD₅₀ (24 hr) dermal ♂, ♀ rat >2000-5000 mg kg⁻¹ (3).

LD₅₀ percutaneous rat >5000 mg kg⁻¹ (1).

LD₅₀ intraperitoneal ♂, ♀ rat 750, 395 mg kg⁻¹, respectively (3).

Sub-acute and sub-chronic data

Dermal ♂, ♀ rabbit (3 wk) 0, 50 or 250 mg kg⁻¹ body weight for 6 hr day⁻¹. No treatment-related effects were observed (3).

Oral ♂, ♀ beagle dogs (13 wk) 0, 200, 1000 or 5000 ppm in diet. The treatment did not affect body temperature, pulse rate or neurological functions and urinalysis showed no treatment-related effects. Food consumption decreased and body-weight gain was retarded in animals given 1000 or 5000 ppm. Administration of 5000 ppm also induced cataracts, elevated the cytochrome P450 content of the liver, increased alkaline phosphatase activity in plasma and produced anisocytosis in 6/8 dogs due to an increase in thrombocyte count. One dog died after being given one dose of 5000 ppm, with no previous clinical signs. The no-observable-adverse-effect level was 200 ppm (3).

Following two one-year studies in dogs a no-observable-adverse-effect level of 100 ppm was determined (3).

Inhalation rats (3 wk) 0, 5, 50 or 500 mg m⁻³ in polyethylene glycol 6 hr day⁻¹, 5 days week⁻¹ had no effect on the mortality rate, body-weight gain or organ weights. No treatment-related gross or histopathological alterations were seen. ♂ and ♀ animals exposed to the highest dose showed increased *N*-demethylase activity; ♂ rats in this group also had increased *O*-demethylase activity. The no-observable-adverse-effect level was 10.6 mg m⁻³ (3).

Carcinogenicity and chronic effects

No-observable-effect level (2 yr) rats, dogs, mice 300, 100, 20 mg kg⁻¹ diet, respectively (1).

Oral ♂, ♀ mice (21 months) 0, 20, 60 or 180 ppm (0, 6, 8 or 53 mg kg⁻¹ day⁻¹). Appearance, behaviour, mortality, food consumption and body weight were not affected, but animals given 180 ppm showed reduced erythrocyte count and haemoglobin and haematocrit values. Sporadic alterations in clinical chemical parameters were observed in all groups. Gross pathological examination showed no treatment-related effects and no increase in tumour incidence was found (3).

In a two-year study, rats were given 0, 100, 300 or 1000 ppm in their diet; no evidence of carcinogenicity was seen. The no-observable-adverse-effect level was 100 ppm (5 mg kg⁻¹ day⁻¹) on the basis of reduced body-weight gain at higher doses (3).

Teratogenicity and reproductive effects

Gavage ♀ rabbits (days 6-18 of gestation) 0, 3, 10 or 30 mg kg⁻¹ day⁻¹. Reproductive and foetal parameters were not adversely affected, and no treatment-related increases in the incidence of malformations were observed.

Animals given the highest dose had reduced body-weight (3).

Gavage ♀ mice (days 6-15 of gestation) 0, 10, 30 or 100 mg kg⁻¹ day⁻¹. Mortality rates, body-weight gain and pregnancy rates were not affected. A dose-related increase in the incidence of runts was seen from dams given ≥30 mg kg⁻¹ day⁻¹ and an increase in malformations (rib fusion, micrognathia, cleft palate and spinal dysplasia) occurred at 100 mg kg⁻¹. The no-observable-adverse-effect level was 100 mg kg⁻¹ day⁻¹ for maternal toxicity and clinical signs and 10 mg kg⁻¹ day⁻¹ for embryotoxicity and teratogenicity (3).

Metabolism and toxicokinetics

After three days, elimination in animals (species not specified) was almost complete (>99%) with the compound being excreted in the urine and faeces (1).

Following oral administration to rats, 65-80% of the dose was eliminated by the biliary and faecal route, with 16-35% being eliminated in the urine. ♂ rats showed greater biliary and faecal elimination than ♀ rats (3). The permeability of human and rat skin *in vitro* was studied using the ¹⁴C-labelled compound. Within 24 hr, 37% of a dose of 1.25 g l⁻¹ in water had permeated human skin, compared with 22% of testosterone and 5% of hydrocortisone (reference compounds). Tebuconazole permeated rat skin more than hydrocortisone, but less than testosterone (3).

Irritancy

Non-irritating to rabbit skin (3).

Instillation of 100 mg into the conjunctival sac of rabbits caused slight irritation of the conjunctiva; 50 mg caused no irritation of the eye (3).

Sensitisation

The compound was found to have no skin-sensitising potential in a maximisation test in guinea pigs (3).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 (metabolic activation unspecified) negative (3).

Escherichia coli WPuvrA with and without metabolic activation negative (3).

In vitro Chinese hamster ovary cells sister chromatid exchange with and without metabolic activation negative (3).

Other effects

Other adverse effects (human)

Workers producing tebuconazole did not show exposure-related effects (3).

Any other adverse effects

In rats, the symptoms of acute poisoning included emaciation, sedation, locomotor uncoordination and spastic gait (3).

Legislation

Included in Schedule 6 (Release Into Land: Prescribed Substances) of Statutory Instrument No. 472, 1991 (4).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides and related products: maximum admissible concentration 0.1 µg l⁻¹ (5).

WHO Toxicity Class III (6).

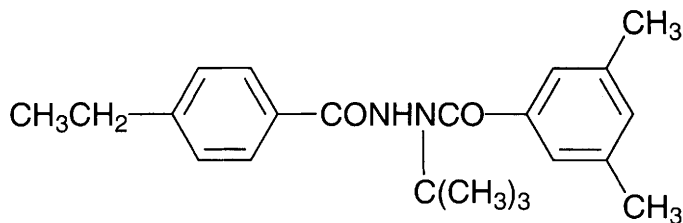
EPA Toxicity Class III (1).

ADI (JMPR) 0.03 mg kg⁻¹ body weight (1).

References

1. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
2. Fritz, R. et al. *Brighton Crop Prot. Conf. – Pest. Dis.* 1992, (2), 829-834.
3. *IPCS Pesticide Residues in Food – Evaluations* 1994, Part II Toxicology, World Health Organisation, Geneva, Switzerland.
4. S.I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations*, 1991, HMSO, London, UK.
5. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
6. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21

T12 tebufenozide



C₂₂H₂₈N₂O₂

Mol. Wt. 352.48

CAS Registry No. 112410-23-8

Synonyms *N*-*tert*-butyl-*N'*-(4-ethylbenzoyl)-3,5-dimethylbenzohydrazide; 3,5-dimethylbenzoic acid 1-(1,1-dimethylethyl)-2-(4-ethylbenzoyl)hydrazide

Uses Ecdysone agonist insecticide used to control defoliating lepidopteran larvae on rice, fruit, row crops, nut crops, vegetables, vines, and forestry.

Physical properties

M. Pt. 191°C **Specific gravity** 1.03 at 20°C **Partition coefficient** log *P*_{ow} 4.25 (pH 7)

Volatility v.p. 2.25×10^{-8} mmHg (25°C, gas saturation method)

Solubility Water: <1 mg l⁻¹. Organic solvents: slightly soluble in organic solvents

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bluegill sunfish, rainbow trout 3.0, 5.7 mg l⁻¹, respectively (1).

Invertebrate toxicity

EC₅₀ (48 hr) *Daphnia magna* 3.8 mg l⁻¹ (1).

LC₅₀ (96 hr) mysid shrimp 1.4 mg l⁻¹ (1).

LC₅₀ earthworm >1000 mg kg⁻¹ (1).

Tebufenozide treatment (0.07-0.66 mg l⁻¹) of large lake enclosures showed a concentration-dependent reduction in the abundance of cladocerans, but no direct toxic effect on copepods or phytoplankton biomass. Recovery of zooplankton communities in the enclosures occurred within 1-2 months at 0.07 and 0.13 mg l⁻¹ and within 12-13 months at 0.33 and 0.66 mg l⁻¹ (2).

Tebufenozide at concentrations up to 100 × the expected environmental concentration resulting from an operational spray rate of 70 g ha⁻¹ did not affect the survival, growth and reproduction of the forest earthworm *Dendrobaena octaedra* in leaf litter over a 10 week period. Population growth over 8-10 weeks in four species of soil Collembola was similarly unaffected (3).

LD₅₀ (96 hr, contact) for honeybees >234 µg bee⁻¹ (1).

Environmental fate

Degradation studies

DT₅₀ 30 days in natural pond water, in light, at 25°C, 100 days for aerobic soil metabolism at 25°C (3 soil types), 175 days for anaerobic aquatic metabolism at 25°C (silt loam), 4-30 days for field dissipation (4 sites) (1).

An emulsion suspension of MIMIC was applied twice over a mixed-wood forest, each time at the rate of 70g active ingredient (tebufenozide) ha⁻¹. The highest concentration of tebufenozide in soil was 0.101 µg g⁻¹ wet weight for the first application and 0.116 µg g⁻¹ for the second application, with DT₅₀ values for the soil of 42.2 and for the litter of 80 days. A stream received very low deposits during the first spray. Maximum 1 hr post-spray concentrations (µg l⁻¹) in the stream (second application) and pond waters (first and second applications) were 1.32, 5.31 and 1.26, respectively, with an average DT₅₀ for all of 1.6 days (4).

Abiotic removal

Stable in dark, sterile water at 25°C for 30 days. Stable at 94°C for 7 days. Stable to light in pH 7 aqueous solution at 25°C (1).

Mammalian & avian toxicity**Acute data**

LD₅₀ oral quail >2150 mg kg⁻¹ (1).

LD₅₀ oral rat, mouse >5000 mg kg⁻¹ (1).

LC₅₀ (4 hr) inhalation ♂ rat 4.3, ♀ rat 4.5 mg l⁻¹ (1).

Sub-acute and sub-chronic data

No-observed-effect level (12 months) dogs 1.9 mg kg⁻¹ body weight daily (1).

Carcinogenicity and chronic effects

No-observed-effect level (24 months) rats 5.5 mg kg⁻¹ body weight daily (1).

No-observed-effect level (18 months) mice 8.1 mg kg⁻¹ body weight daily (1).

Irritancy

Non-irritating to eyes and skin of rabbits (1).

Sensitisation

Tebufenozide does not sensitise the skin of guinea pigs (1).

Genotoxicity

Ames test, reverse mutation assay, mammalian point mutation (CHO), *in vivo* and *in vitro* cytogenetic assay, and unscheduled DNA synthesis assay negative (1).

Legislation

EPA Toxicity Class III (formulation) (1).

ADI 0.019 mg kg⁻¹ body weight (1).

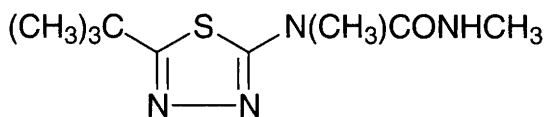
Other comments

Non-phytotoxic (1).

References

1. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
2. Kreutzweiser, D. P. et al *Ecotoxicology* 1995, 4(5), 307-328.
3. Addison, J. A. *Ecotoxicol. Environ. Saf.* 1996, 33(1), 55-61.
4. Sundaram, K. M. S. et al *J. Environ. Sci. Health, Part B* 1996, B31, 699-750

T13 tebuthiuron



C₉H₁₆N₄OS

Mol. Wt. 228.32

CAS Registry No. 34014-18-1

Synonyms N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-N,N'-dimethylurea; 1-(5-*tert*-butyl-1,3,4-thiadiazol-2-yl)-1,3-dimethylurea; EL-103; Graslan; Spike

EINECS No. 251-793-7

RTECS No. YS 4250000

Uses Herbicide.

Physical properties

M. Pt. 161.5-164°C (decomp.) **Partition coefficient** log P_{ow} 1.78 **Volatility** v.p. 2.025 × 10⁻⁶ mmHg at 25°C
Solubility Water: 2.5 g l⁻¹ at 25°C. Organic solvents: acetone, acetonitrile, benzene, chloroform, hexane, methanol, methoxyethanol

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed (R22)

Safety phrases Keep out of reach of children (if sold to general public) – Wear suitable gloves (S2, S37)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bluegill sunfish, trout, goldfish and fathead minnow 112-160 mg l⁻¹ (1).

Invertebrate toxicity

EC₅₀ (5 min) *Photobacterium phosphoreum* 330 ppm, Microtox test (2).

Tebuthiuron poses a low acute exposure risk to *Selenastrum capricornutum* (3).

EC₅₀ *Selenastrum capricornutum* 0.08 mg l⁻¹ (4).

EC₅₀ *Photobacterium phosphoreum* 328 mg l⁻¹ (4).

LD₅₀ >100 µg bee⁻¹ (1).

Environmental fate

Nitrification inhibition

It reduced nitrification in all soils at 1000 µg g⁻¹. An increased net mineralisation was observed when it was added at 100 and 1000 µg g⁻¹ (5).

Degradation studies

The t_{1/2} is soil in 12-15 months. Persistence in soil is inversely related to the soil moisture content, which corresponds with the humus content (1).

Degradation of 20 µg g⁻¹ soil occurred within 160 days (6).

It did not exhibit bioactivity after 14 months from its application at 1.2 kg ha⁻¹ (7).

Adsorption and retention

Freundlich K values range from 0.11 in sand to 1.82 in clay loam (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral cat, rabbit, dog, mouse, rat 200-644 mg kg⁻¹ (1,8,9).

Irritancy

Dermal rabbit (unspecified duration) 200 mg kg⁻¹ or 71 mg kg⁻¹ instilled into rabbit eye did not cause irritation (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (10).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (11).

WHO Toxicity Class III (12).

EPA Toxicity Class III (formulation) (1).

ADI 0.07 mg kg⁻¹ daily (based on two-generation rat reproduction study) (1).

Other comments

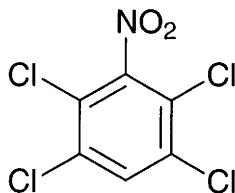
At 3.36 kg ha⁻¹ it was most effective at pre-emergence control of *Cynodon nemfuensis* (13).

Metabolic pathways reviewed (14).

References

1. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
2. Kaiser, K. L. E. *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
3. Blaise, C. et al *Rev. Sci. Eau* 1991, **4**(1), 121-134.
4. Hickey, C. W. et al *Environ. Toxicol. Water Qual.* 1991, **6**(40), 383-403.
5. Goodroad, L. L. *Commun. Soil Sci. Plant Anal.* 1987, **18**(4), 473-481.
6. Raman, S. et al *Toxicol. Environ. Chem.* 1987, **15**(4), 265-272.
7. Oliveria, D. A. *Pesqui. Afropecu. Bras.* 1987, **22**(7), 681-687 (Port.).
8. *Farm Chemicals Handbook* 1980, D286, Meister Publishing, Willoughby, OH, USA.
9. *Wirksubstanzen der Pflanzenschutz- und Schaedlingsbekaempfungsmittel* 1971, Verlag Paul Parey, Berlin, Germany.
10. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
11. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
12. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
13. Lugo, M. L. et al *J. Agric. Univ. P. R.* 1989, **73**(2), 149-153.
14. Roberts, T. R. et al (Eds.) *Metabolic Pathways of Agrochemicals. Part 1: Herbicides and Plant Growth Regulators* 1998, The Royal Society of Chemistry, Cambridge, UK

T14 tecnazene



C₆HCl₄NO₂

Mol. Wt. 260.89

CAS Registry No. 117-18-0

Synonyms Arena; Bygran; Fusarex; Hystore; Nebulin; 1,2,4,5-tetrachloro-3-nitrobenzene; Tubodust; benzene, tetrachloronitro-; 2,3,5,6-tetrachloro-1-nitrobenzene

EINECS No. 204-178-2

RTECS No. DC 0175000

Uses Fungicide. Plant growth regulator.

Physical properties

M. Pt. 99°C **B. Pt.** 304°C (decomp.) **Specific gravity** 1.744 at 25°C with respect to water at 4°C

Partition coefficient log *P*_{ow} 3.98 (1) **Volatility** v.p. 1.80 × 10⁻³ mmHg at 15°C

Solubility Water: 0.44 mg l⁻¹ at 20°C. Organic solvents: acetone, benzene, carbon disulfide, chloroform, ethanol

Occupational exposure

Supply classification irritant

Risk phrases May cause sensitisation by skin contact (R43)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with the skin – Wear suitable gloves (S2, S24, S37)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) rainbow trout, stickleback, eel 370-1400 µg l⁻¹ (2).

Invertebrate toxicity

LC₅₀ (96 hr) *Gammarus pulex*, *Asellus aquaticus* 270, 1060 µg l⁻¹, respectively (2).

LC₅₀ (96 hr) *Limnaea peregra* 570-2300 µg l⁻¹ (2).

EC₅₀ (30 min) *Photobacterium phosphoreum* 8.3 ppm Microtox test (3).

Non-toxic to bees (4).

Bioaccumulation

Bioconcentration factor 2400-5200 in rainbow trout (2).

Environmental fate

Degradation studies

Biodegradation 8% after 60 days; 21% after 128 days; 26% after 240 days; 24% after 300 days incubation at 25°C (5).

Degradation *t*_{1/2} 0.1 days in screening study utilising anaerobic sewage, sludge inoculum. The major degradation product was 2,3,5,6-tetrachloroaniline (6).

Abiotic removal

Reaction with photochemically produced hydroxyl radicals in the atmosphere *t*_{1/2} 93 days (7).

Rapidly lost from soil mainly through evaporation (8).

Volatilisation *t*_{1/2} 2.8 days in model river water, 31 days in model pond water if adsorption to sediments ignored (9,10).

Adsorption and retention

Estimated K_{oc} of 3500 indicates that tecnazene will adsorb to soil and sediments (9).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 7500 mg kg⁻¹ (11).

Sub-acute and sub-chronic data

Oral rat 2000 mg kg⁻¹ diet for 10 wk caused no effects other than increased liver and testes weight in ♂ rats (12).

Carcinogenicity and chronic effects

Oral rat (2 yr) 150 mg kg⁻¹ diet caused no carcinogenic response (8).

Oral mouse (560 day) 1500 mg kg⁻¹ diet caused no carcinogenic response (8).

Teratogenicity and reproductive effects

In a two-generation study, rats were administered 0, 200, 800 or 3200 mg kg⁻¹ diet for 12 wk in each generation prior to mating. No adverse reproductive effects were observed; maternal growth rate was slightly retarded in the high-dose group (13).

Oral rat, mouse 200 mg day⁻¹ on days 7-18 of gestation in rats and 7-16 in mice, caused no foetotoxic or teratogenic effects (14).

Metabolism and toxicokinetics

Following oral administration to mammals, rapidly absorbed and metabolised. The most important urinary metabolite is the mercapturic acid conjugate. High single doses are predominantly excreted unchanged in the urine (8).

Irritancy

Irritating to the skin, eyes, mucous membranes and upper respiratory tract (species unspecified) (15).

Sensitisation

Dermal sensitisation had been reported among exposed agricultural workers (16).

Genotoxicity

Salmonella typhimurium TA100 with metabolic activation negative (17).

Aspergillus niger dominant lethal mutation with metabolic activation aneuploidy and crossing over positive (18).

Drosophila melanogaster sex-linked recessive lethal assay negative (19).

In vitro Chinese hamster ovary cells sister chromatid exchanges weakly positive, chromosomal aberrations negative (metabolic activation unspecified) (20).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (21).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (22).

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th Amendments) (23).

WHO Toxicity Class Table 5 (24).

ADI (JMPR) 0.02 mg kg⁻¹ body weight (4).

Other comments

Residues have been isolated from crops and soils (13).

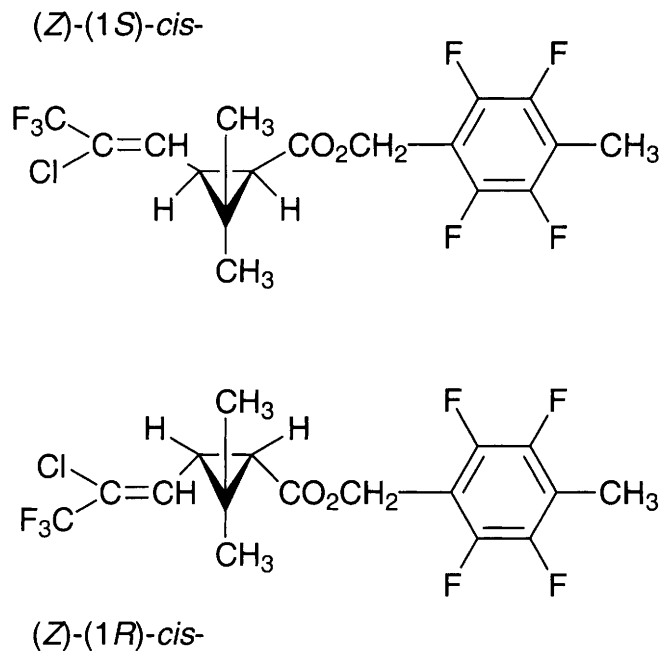
Physical properties, use, occurrence, environmental fate and toxicity reviewed (13).

Metabolic pathways reviewed (25).

References

1. Hansch, C. et al *Medchem. Project Issue No. 26* 1985, Pomona College, Claremont, CA, USA.
2. Whale, G. et al *Chemosphere* 1988, **17**(6), 1205-1217.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
5. Caseley, J. C. et al *Bull. Environ. Contam. Toxicol.* 1968, **3**, 180-191.
6. Geer, R. D. et al *Predicting the Anaerobic Degradation of Organic Chemicals, Pollutants in Waste Water Treatment Plants from their Environmental Reduction Behaviour* 1978, Bozman, M. T., NTIS PB-289224.
7. Niimi, A. J. et al *Environ. Toxicol. Chem.* 1989, **8**, 817-823.
8. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
9. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behaviour of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
10. *EXAMS II Computer Simulation* 1987, US EPA, Athens, GA, USA.
11. Perkow, W. *Wirksubstanzen der Pflanzenschutz- und Schaedlingsbekaempfungsmittel* 1971-76, Verlag Paul Parey, Berlin, Germany.
12. Wit, S. L. et al *Proc. 4th Int. Crop Protect., Hamburg* 1954, **2**, 1665-1668.
13. *IPCS Environmental Health Criteria No. 42: Tecnazene* 1984, WHO, Geneva, Switzerland.
14. Courtney, K. D. et al *Toxicol. Appl. Pharmacol.* 1976, **35**, 239-256.
15. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3248, Sigma-Aldrich, Milwaukee, WI, USA.
16. Luperknova, K. A. et al *Gig. Tr. Prof. Zabol.* 1965, **9**, 56-58.
17. Klopman, G. et al *J. Comput. Chem.* 1988, **9**(3), 232-243.
18. *GENE-TOX Program: Current Status of Bioassay in Genetic Toxicology* US EPA, Washington, DC, USA.
19. Yoon, Y. S. et al *Environ. Mutagen.* 1985, **7**(3), 349-367.
20. Galloway, S. M. et al *Environ. Mol. Mutagen.* 1987, **10**(Suppl. 10), 1-175.
21. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
22. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
23. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; *6th Amendment EEC Directive* 79/831/EEC; *7th Amendment EEC Directive* 91/32/EEC 1991, HMSO, London, UK.
24. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
25. Roberts, T. R. et al (Eds.) *Metabolic Pathways of Agrochemicals. Part 1: Herbicides and Plant Growth Regulators* 1998, The Royal Society of Chemistry, Cambridge, UK

T15 tefluthrin



$C_{17}H_{14}ClF_7O_2$

Mol. Wt. 418.74

CAS Registry No. 79538-32-2

Synonyms 2,3,5,6-tetrafluoro-4-methylbenzyl (Z)-(1RS, 3RS)-3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethylcyclopropanecarboxylate; [1 α ,3 α (Z)]-(\pm)-(2,3,5,6-tetrafluoro-4-methylphenyl)methyl 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethylcyclopropanecarboxylate; téfluthrine

Uses Insecticide used in the control of a wide range of soil insect pests, particularly those of the orders Coleoptera, Lepidoptera, and Diptera in maize, sugar beet and other crops.

Physical properties

M. Pt. 44.6°C (tech. 39–43 °C) **B. Pt.** 153°C at 1 mmHg **Flash point** 124°C **Specific gravity** 1.48 g ml⁻¹ at 25°C **Partition coefficient** log P_{ow} 6.5 (20°C) **Volatility** v.p. 6×10^{-5} mmHg

Solubility Water: 0.02 mg l⁻¹ (purified and buffered, pH 5 and 9, 20°C). Organic solvents: acetone, dichloromethane, ethyl acetate, hexane, methanol, toluene

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) rainbow trout, bluegill sunfish 60, 130 ng l⁻¹, respectively (1).

Invertebrate toxicity

EC₅₀ (48 hr) *Daphnia magna* 70 ng l⁻¹ (1).

LD₅₀ (contact) 280 ng bee⁻¹, (oral) 1880 ng bee⁻¹ (1).

There were no effects on soil microflora following an even incorporation of tefluthrin to give 1 mg active ingredient kg⁻¹ soil (equivalent to an excessive field rate of 1 kg active ingredient ha⁻¹). A band application of granules at the rate of 112.5 g active ingredient ha⁻¹ had no effect on populations of earthworms in the field (2).

Environmental fate

Degradation studies

Tefluthrin was readily degraded ($t_{1/2}$ 3-20 wk) in all except sterile soil in laboratory tests. Under field conditions tefluthrin was degraded with $t_{1/2}$ approximately 4 wk (3).

Abiotic removal

Stable to hydrolysis at pH 5-7 for >30 days. At pH 9, 7% hydrolysis in 30 days. At pH 7, 27-30% loss in aqueous solution exposed to sunlight for 31 days (1).

Volatilisation of the active ingredient from soil-incorporated granules was not an important dissipation mechanism (3).

Adsorption and retention

Field studies showed that tefluthrin did not leach below 20 cm (3).

Mammalian & avian toxicity

Acute data

LD₅₀ bobwhite quail, mallard duck 730, 4190 mg kg⁻¹, respectively (1).

LD₅₀ ♂ and ♀ rat 22, 35 mg kg⁻¹, respectively (1).

LD₅₀ mouse 45-46 mg kg⁻¹ (1).

LD₅₀ dermal ♂ rats 148-1480 mg kg⁻¹, ♀ rats 262 mg kg⁻¹ (1).

LD₅₀ dermal rabbit >2000 mg kg⁻¹ (1).

LC₅₀ inhalation (4 hr) rat 0.0427 mg l⁻¹ (1).

Carcinogenicity and chronic effects

No-observed-effect level (2 yr) rat 25 mg kg⁻¹ in diet (1).

No-observed-effect level (1 yr) dog 0.5 mg kg⁻¹ daily (1).

Metabolism and toxicokinetics

A goat was dosed twice daily for 4 days at a rate equal to 10.9 mg kg⁻¹ in its diet. Within 16 hr of the final dose 70.1% of the dose had been excreted (urine 41.4% and faeces 28.7%). Extensive metabolism occurred by ester cleavage and oxidation at a variety of positions on the molecule (4).

Irritancy

Caused slight eye and skin irritation in rabbits (1).

Sensitisation

Not a skin sensitising agent for guinea pigs (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (5).

Included in Schedule 6 (Release into Land: Prescribed Substances) of Statutory Instrument No. 472, 1991 (6).

The US Federal Food, Drug, and Cosmetic Act sets a provisional tolerance of 0.06 ppm for tefluthrin and its metabolites, (Z)-3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethylcyclopropanecarboxylic acid and 2,3,5,6-tetrafluoro-4-hydroxymethylbenzoic acid in or on field corn and popcorn grain, forage, and fodder (7).

WHO Toxicity Class Ib (8).

Other comments

Non-phytotoxic to crops when used as recommended (1).

Maize and sugar beet plants grown in soil treated with a granular application of tefluthrin were found to contain pesticide residues in the foliage (0.01-0.46 mg kg⁻¹). Sugar beet roots contained 0.04 mg kg⁻¹. The residues were mainly free and conjugated metabolites of tefluthrin (9).

1. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
2. Coulson, J. M. et al *Brighton Crop Prot. Conf. – Pests Dis.*, 1990, (3), 975-980.
3. Bewick, D. W. et al *Proc. – Br. Crop Prot. Conf. – Pests Dis.* 1986, (2), 459-468.
4. Heath, J. et al *Pestic. Sci.* 1989, 25(4), 375-389.
5. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
6. *S.I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
7. *Fed. Regist.* 1989, 54(20), 5080-5081.
8. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
9. Amos, R. et al *Proc. – Br. Crop Prot. Conf. – Pests Dis.* 1986, (2), 821-828

Te

Physical properties

Occupational exposure

Mammalian & avian toxicity

LD₅₀ oral mouse, guinea pig, rabbit, rat 20-83 mg kg⁻¹ (form of tellurium unspecified) (1).

Oral rat (duration unspecified) 1.1% in feed caused a highly synchronous primary demyelination of peripheral nerves, followed closely by a period of remyelination (2).

Oral neonatal rats (dose unspecified) from day of birth until sacrifice at 7, 14, 21 and 28 days of age. Schwann cell and myelin degeneration were observed. In the central nervous system, hypomyelination of the optic nerve was demonstrated at 14, 21 and 28 days of age, with evidence of myelin degeneration (3).

Teratogenesis characterised by hydrocephalus has been reported following the administration of tellurium to rats (4).

Subcutaneous Wistar rat 0-1000 $\mu\text{mol kg}^{-1}$ in olive oil from day 15-19 of gestation. External and internal examinations were performed on day 20 fetuses. Doses of $>10 \mu\text{mol kg}^{-1}$ resulted in a dose-related appearance of hydrocephalus, oedema, exophthalmia, ocular haemorrhage, umbilical hernia, undescended testes and small kidneys (5,6).

Oral pregnant rats 0, 30, 300, 3000, or 15,000 ppm on days 6-15 of gestation, and artificially inseminated rabbits 0, 17.5, 175, 1750 or 5250 ppm on days 6-18 of gestation. Signs of maternal toxicity were observed during the treatment in a dose-related manner at ≥ 300 ppm in rats and 1750 ppm in rabbits. No effects on reproduction as measured by pregnancy rate, litter size, dead or reabsorbed implantation or foetal sex ratio. Rabbit fetuses at the highest dosage groups had a slightly elevated evidence of skeletal delays and nonspecific abnormalities (7).

Metabolism and toxicokinetics

It is poorly absorbed by humans (8).

When absorbed, a garlic-like odour is evident which is attributed to dimethyltelluride in the breath and sweat.

Normal concentration in the urine is 0.2-1.0 $\mu\text{g l}^{-1}$ (9).

When injected intracerebrally it is found in the grey matter and not the white matter (10).

It has been detected in human scalp hair (11).

In oral rats administered 1.1% elemental tellurium, cholesterol synthesis was severely inhibited and labelled squalene was accumulated in the sciatic nerve after 12 hr exposure (8).

Other effects

Other adverse effects (human)

Exposure of iron foundry workers to concentrations of 0.01-0.1 mg m^{-3} for 22 months produced mild gastro-intestinal distress, the characteristic garlic odour, dryness of the mouth, metallic taste and somnolence (9).

Other comments

Air concentration of tellurium-containing dusts was 0.4-181 mg m^{-3} at a Russian factory (12).

Toxicity in humans and laboratory animals, and its nature as a pollutant, reviewed (13,14).

References

1. Izmerov, N. F. *Toxicometric Parameters of Industrial Toxic Chemicals Under Single Exposure* 1982, 105.
2. Bouldin, T. W. et al *Neurotoxicology* 1989, 10, 79.
3. Jackson, K. F. et al *Acta Neuropathol.* 1989, 78(3), 310-319.
4. Dockett, S. *Experientia* 1970, 26, 83.
5. Perez-D'Gregorio, R. E. et al *Teratology* 1988, 37(4), 307-316.
6. Perez-D'Gregorio, R. E. et al *Reprod. Toxicol.* 1988, 2(1), 55-61.
7. Johnson, E. M. et al *Fundam. Appl. Toxicol.* 1988, 11(4), 691-702.
8. *Patty's Industrial Hygiene and Toxicology* 3rd rev. 1981, John Wiley & Sons, New York, NY, USA.
9. Steinberg, H. H. et al *J. Ind. Hyg. Toxicol.* 1942, 24, 183.
10. Thienes, C. et al *Clinical Toxicology* 5th ed., 1972, 199, Lea and Febeger, PA, USA.
11. Lal, G. et al *Nucl. Med. Biol.* 1987, 14(5), 499-501.
12. Altynbekov, B. E. et al *Vestn. Akad. Nauk. Kaz. SSR* 1988, (90), 60-65.
13. Srivastava, S. et al *J. Recent Adv. Appl. Sci.* 1987, 2(1), 267-271.
14. Hashimoto, Y. *Bunseki* 1990, (2), 111-117

T17 tellurium hexafluoride



F₆Te

Mol. Wt. 241.59

CAS Registry No. 7783-80-4

EINECS No. 232-027-0

RTECS No. WY 2800000

Physical properties

M. Pt. -37.6°C B. Pt. sublimates at -38.9°C Specific gravity 4.006 at -191°C (solid), 2.499 at -10°C (liquid)

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Te) (inhalable fraction of aerosol)

FR-VME 0.02 ppm (0.2 mg m⁻³) (as Te)

SE-LEVL 0.1 mg m⁻³ (as Te)

UK-LTEL 0.1 mg m⁻³ (as Te)

US-TWA 0.02 ppm

UN No. 2195 Conveyance classification toxic gas, corrosive

Environmental fate

Abiotic removal

Hydrolysed in water to telluric acid.

Mammalian & avian toxicity

Acute data

LC₅₀ (24 hr) inhalation rat mouse 5 ppm (1).

LC_{Lo} (8 hr) inhalation rabbit, guinea pig 5 ppm (1).

Other effects

Other adverse effects (human)

Two cases of excessive occupational exposure have been reported. Because both workers were also handling volatile liquid esters, some increased absorption and deposition of elemental tellurium in the skin may have occurred. The signs included garlic breath. An unusual feature was bluish-black discoloration of the webs of the fingers and streaks on the face and neck. No permanent damage was noted (2).

Any other adverse effects

It is considered toxic by inhalation and may produce pulmonary oedema and death (species unspecified) (3).

References

1. *Archiv fuer Toxikologie* 1960, 18, 140.
2. Blackadder, E. S. et al *Brit. J. Ind. Med.* 1975, 32, 59.
3. *Patty's Industrial Hygiene and Toxicology* 1981, 3rd rev. ed., John Wiley & Sons, New York, NY, USA

T18 tellurium tetrachloride



Cl_4Te

Mol. Wt. 269.41

CAS Registry No. 10026-07-0

Synonyms telluric chloride

EINECS No. 233-055-6

RTECS No. WY 2635000

Physical properties

M. Pt. 224°C B. Pt. 380°C Specific gravity 3.26

Solubility Water: decomposes. Organic solvents: ethanol, toluene

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Te) (inhalable fraction of aerosol)

FR-VME 0.1 mg m⁻³ (as Te)

SE-LEVL 0.1 mg m⁻³ (as Te)

UK-LTEL 0.1 mg m⁻³ (as Te)

US-TWA 0.1 mg m⁻³ (as Te)

UN No. 3284 HAZCHEM Code 2X Conveyance classification toxic substance

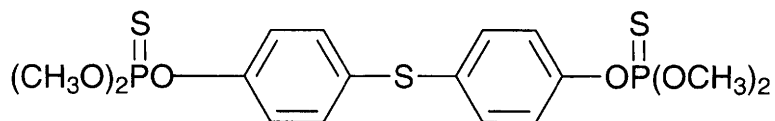
Other comments

Applications of tellurium tetrachloride in the rubber industry are reviewed (1).

References

1. Akiba, M. *Porima Daijesuto* 1988, 40(12), 43-52

T19 temephos



$\text{C}_{16}\text{H}_{20}\text{O}_6\text{P}_2\text{S}_3$

Mol. Wt. 466.48

CAS Registry No. 3383-96-8

Synonyms Abate; Abathion; Biothion; Nimitex; *O,O,O',O'*-tetramethyl *O,O'*-thiodi-*p*-phenylene-diphosphorothioate; *O,O'*-(thiodi-4,1-phenylene) bis(*O,O*-dimethylphosphorothioate); *O,O'*-thiodi-*p*-phenylene *O,O,O',O'*-tetramethyl bis(phosphorothioate)

EINECS No. 222-191-1

RTECS No. TF 6890000

Uses Insecticide.

Physical properties

M. Pt. 30-30.5°C **Flash point** 43-93°C (closed cup) **Specific gravity** 1.32 (tech.) **Partition coefficient** $\log P_{ow}$ 4.9079 (1)

Solubility Water: 0.03 mg l⁻¹ at 25°C. Organic solvents: acetonitrile, benzene, chloroform, diethyl ether, toluene

Occupational exposure

FR-VME 10 mg m⁻³

US-TWA 10 mg m⁻³

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) mosquito fish 5.6 mg l⁻¹ (2).

LC₅₀ (96 hr) mummichog 0.04 mg l⁻¹ (3).

Perch exposed to 10 mg l⁻¹ exhibited an immediate reduction in ventilation rate and oxygen consumption, and reduced heart rate during the 2nd hour of exposure. All fish died within 12 hr (4).

Invertebrate toxicity

LD₅₀ topical bee 1.6 µg bee⁻¹ (1).

LC₅₀ (96 hr) *Gammarus lacustris* 82 µg l⁻¹ (5).

LC₅₀ (72 hr) *Metapenaeus moroceros*, *Penaeus meerodon* 45 µg l⁻¹ static bioassay (6).

Environmental fate

Abiotic removal

Undergoes hydrolysis at pH >2 and <9 (7).

Adsorption and retention

Soil adsorption Freundlich K 73 in loamy sand, 130 in sandy loam, 244 in silt loam, 540 in loam (7).

Mammalian & avian toxicity

Acute data

LD₅₀ oral ♂, ♀ rat 8600, 13,000 mg kg⁻¹, respectively (1).

LD₅₀ oral redwing blackbird, quail 42, 75 mg kg⁻¹, respectively (8).

LD₅₀ oral mouse, rabbit 223, 313 mg kg⁻¹, respectively (9,10).

LD₅₀ dermal rabbit 970 mg kg⁻¹ (11).

LD₅₀ intraperitoneal rat 912 mg kg⁻¹ (12).

LD₅₀ subcutaneous rat 2302 mg kg⁻¹ (12).

Sub-acute and sub-chronic data

LC₅₀ (5 day) oral ring-necked pheasant, mallard duck 170, 1200 mg kg⁻¹ diet, respectively (1).

Carcinogenicity and chronic effects

Oral rat (2 yr) no-adverse-effect level 300 mg kg⁻¹ (1).

Teratogenicity and reproductive effects

Dermal rabbit, lowest toxic dose 2100 mg kg⁻¹ day⁻¹ on days 6-18 of gestation (foetotoxicity) (13).

Metabolism and toxicokinetics

In mammals, principally eliminated unchanged in the faeces and urine. Urinary metabolites include sulfate esters of 4,4'-thiodiphenol, 4,4'-sulfinyldiphenol, and 4,4'-sulfonyldiphenol (1).

Irritancy

Dermal rabbit (24 hr) 500 mg caused mild irritation (14).

Other effects

Other adverse effects (human)

Oral man, 260 mg subject⁻¹ day⁻¹ for 5 days, or 64 mg subject⁻¹ day⁻¹ for 28 days caused no toxic effects (15).

Any other adverse effects

Inhibits cholinesterase (1).

Intraperitoneal rat, single doses of 310, 560 or 1000 mg kg⁻¹. The high dose caused impaired performance of previously conditional avoidance response 6 days after injection, but not at 2, 8, 10 or 16 days after injection (16).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (17).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (18).

The log P_{ow} value exceeds the European Community recommended level of 3.0 (Directive on Classification, Packaging and Labelling Dangerous Substances, 6th and 7th Amendments (19).

WHO Toxicity Class Table 5 (20).

EPA Toxicity Class III (formulation) (7).

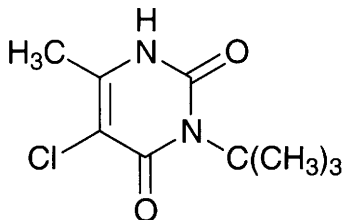
Other comments

Metabolism in plants involves oxidation to the sulfoxide, and, to a lesser extent, the sulfone and the mono- and di-orthophosphates. Further degradation proceeds very slowly (1).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. Tietze, N. S. et al *J. Am. Mosq. Control Assoc.* 1991, 7(2), 290-293.
3. Lee, B. M. et al *Bull. Environ. Contam. Toxicol.* 1989, 43(6), 827-832.
4. Gelarke, P. C. et al *Aust. J. Mar. Freshwater Res.* 1988, 39(6), 767-774.
5. Sander, H. O. *Toxicity of Pesticides to the Crustacean, Gammarus lacustris* 1969, Bureau of Sport Fisheries and Wildlife Technical Paper 25, Washington, DC, USA.
6. Tsai, S. C. *Trans. Am. Fish Soc.* 1978, 107, 493.
7. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
8. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, 12, 355-382.
9. Agricultural Research Service *USDA Inf. Mem.* 1966, 20, 1.
10. *Veterinariya* 1984, 60(11), 63.
11. *Toxicological Information on Cyanamid Insecticides* 1966, American Cyanamid Co., Princeton, NJ, USA.
12. *Toho Igakkai Zasshi* 1969, 16, 297.
13. Report No. AD-A134-545, National Technical Information Service, Springfield, VA, USA.
14. *Toxicol. Appl. Pharmacol.* 1972, 21, 369.
15. Laws, R. L. et al *Arch. Environ. Health* 1967, 14, 289.
16. Kurtz, P. J. et al *Toxicology* 1979, 13(1), 35-44.
17. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
18. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
19. 1967 *Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
20. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21

T20 **terbacil**



C₉H₁₃ClN₂O₂

Mol. Wt. 216.67

CAS Registry No. 5902-51-2

Synonyms 3-*tert*-butyl-5-chloro-6-methyluracil; 5-chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1*H*,3*H*)-pyrimidinedione; Geonter; Sinbor

EINECS No. 227-595-1

RTECS No. YQ 9360000

Uses Herbicide.

Physical properties

M. Pt. 175-177°C **B. Pt.** sublimation begins below the melting point **Specific gravity** 1.34 at 25°C with respect to water at 25°C **Partition coefficient** log *P*_{ow} 1.91 (1) **Volatility** v.p. 4.7×10^{-7} mmHg at 30°C
Solubility Water: 710 mg l⁻¹ at 25°C. Organic solvents: butyl acetate, cyclohexanone, dimethylformamide, methyl isobutyl ketone, xylene

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) pumpkinseed sunfish 86 mg l⁻¹ (2).

Invertebrate toxicity

LC₅₀ (48 hr) fiddler crab >1000 mg l⁻¹ (2).

Non-toxic to bees (3).

Environmental fate

Degradation studies

Undergoes microbial degradation in moist soil. Degradation *t*_{1/2} 5-8 months in top soil after application of 4.5 kg ha⁻¹ (4).

<5% degradation in 60 days in anaerobic silt loam and sandy soils (5).

Abiotic removal

16% degradation by UV irradiation at 300-400 nm in distilled water after 4 wk (6).

Adsorption and retention

Negligibly adsorbed to soils ranging in texture from sand to clay. 54% adsorption to muck soil containing 36% organic matter (6-8).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 5000-7500 mg kg⁻¹ (9).

Sub-acute and sub-chronic data

LC₅₀ (8 day) oral Pekin duckling >56 g kg⁻¹ diet, pheasant chicks 31.5 g kg⁻¹ diet (1,10).

Dermal rabbit 5000 mg kg⁻¹ day⁻¹, 5 hr day⁻¹, 5 days wk⁻¹ for 3 wk caused no toxic effects (10).

Carcinogenicity and chronic effects

Oral mouse 0, 7.5, 180 or 750 (increased to 1100) mg kg⁻¹ day⁻¹ for 2 yr. The high dose caused increased mortality. An increased incidence of hepatocellular hypertrophy was seen in ♂ and ♀ mice administered the high dose and in ♂ mice administered 180 mg kg⁻¹ (11).

Oral rat 0, 2.5, 12.5 or 125 (increased to 500) mg kg⁻¹ day⁻¹ for 2 yr. Rats administered the high dose exhibited a significantly reduced body-weight gain and a slight increase in liver weight. Histological changes were observed in the livers of mid- and high-dose groups. These changes consisted of enlargement and occasional vacuolation of centrilobular hepatocytes (12).

Teratogenicity and reproductive effects

Oral rat 0, 2.5 or 12.5 mg kg⁻¹ day⁻¹ for 100 days prior to mating, for three generations. ♂ rats administered the high dose exhibited reduced body-weight gain. No abnormalities in fertility, and no foetotoxic or teratogenic effects were observed (13).

Gavage rabbit 0, 30, 200 or 600 mg kg⁻¹ day⁻¹ on days 7-19 of gestation. Maternal and foetal toxicity was reported with the high dose, evidenced by reduced weight gain. The high dose also caused a statistically insignificant increase in the frequency of extra ribs and partially ossified phalanges. This suggests that these effects may have been the result of maternal toxicity (14).

Oral rat 0, 20, 100 or 400 mg kg⁻¹ day⁻¹ on days 6-15 of gestation. Reduced food consumption and body-weight gain were observed in the two higher-dose groups. The mean number of live foetuses was also significantly reduced in these groups. Developmental effects observed were anomalies in the renal pelvis and ureter dilation in all treated groups (15).

Metabolism and toxicokinetics

In mammals, the principal biotransformation involves hydroxylation of the 6-methyl group, and replacement of the 5-chloro group with a hydroxy group (16).

Irritancy

Mild eye irritant to rabbits but no skin irritation to rabbits and guinea pigs at 5000 mg kg⁻¹ (10,17).

Sensitisation

No skin sensitisation was observed in guinea pigs (18).

Genotoxicity

Drosophila melanogaster sex-linked recessive lethal assay negative (19).

In vitro Chinese hamster ovary cells sister chromatid exchanges negative (metabolic activation unspecified) (19).

In vitro Chinese hamster ovary cells HGPRT assay with and without metabolic activation negative (20).

In vitro rat primary hepatocytes unscheduled DNA synthesis negative (20).

In vivo rat bone marrow cells chromosomal aberrations negative (20).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (21).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (22).

WHO Toxicity Class Table 5 (23).

EPA Toxicity Class IV (formulation) (3).

Other comments

Physical properties, environmental fate, mammalian toxicity, teratogenicity, mutagenicity, carcinogenicity, health advisories and analytical methods reviewed (1).

Photosynthetic electron transport inhibitor (3).

Metabolic pathways reviewed (24).

References

1. *Drinking Water Health Advisory: Pesticides* 1988, 743-757, USEPA Office of Drinking Water Health Advisories, Lewis Publishers, Chelsea, MI, USA.
2. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
3. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
4. Marriage, P. B. *Weed Res.* 1977, 17, 219-255.
5. Rhodes, R. C. *Report* 1975, du Pont de Nemours Co. Inc., Wilmington, DE, USA.
6. Davidson, J. M. et al *Report* 1978, EPA 600/9-78-016, 233-244, Washington, DC, USA.
7. Liu, L. C. et al *J. Agric. Univ. Puerto Rico* 1971, 5(4), 451-460.
8. Rao, P. S. C. et al *Water Res.* 1979, 13, 375-380.
9. Sherman, H. *Oral LD₅₀ Test* 1965 Report No. 160-65, MRID 00012235, E.I. du Pont de Nemours Co. Inc., Newark, DE, USA.
10. Hood, D. *Report* 1965, Report No. 33-66, MRID 000125785.
11. Goldenthal, E. S. et al *Two-Year Feeding Study in Mice (Terbacil)* 1981, International Research and Development Corp. No. 125-100, MRID 0126770.
12. Wazeter, F. X. et al *Two-Year Feeding Study in the Albino Rat* 1967, International Research and Development Corp. No. 125-100, MRID 0060850.
13. Wazeter, F. X. et al *Three-Generation Reproduction Study in the Rat* 1967, International Research and Development Corp. No. 125-012, MRID 0060852.
14. *Embryo-Foetal Toxicity and Teratogenicity Study of Terbacil by Gavage in the Rabbit* 1984, E. I. du Pont de Nemours Co. Inc., Newark, DE, USA.
15. Culick, R. et al *Teratology Study in Rats* 1980, Haskel Laboratory Report No. 481-79, Newark, DE, MRID 0050467.
16. Mayo, B. C. et al *Proc. Brighton Crop Protection Conf. – Pests Dis.* 1988, 2, 681.
17. Clayton, G. D. et al (Eds.) *Patty's Industrial Hygiene and Toxicology* 3rd ed., 1981, 2A, 2749.
18. Reinke, R. E. *Report* 1965, Report No. 79-65, E. I. du Pont de Nemours Co. Inc., Newark, DE, MRID 0006803.
19. Borzonyi, M. et al *Acta Morphol. Hung.* 1987, 35(1-2), 3-8.
20. *In Vitro Testing of Terbacil* 1984, E. I. du Pont de Nemours Co. Inc., Newark, DE, USA.
21. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
22. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
23. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
24. Roberts, T. R. et al (Eds.) *Metabolic Pathways of Agrochemicals. Part 1: Herbicides and Plant Growth Regulators* 1998, The Royal Society of Chemistry, Cambridge, UK

T21 terbium

Tb

Tb

Mol. Wt. 158.93

CAS Registry No. 7440-27-9

EINECS No. 231-137-6

Uses As magnetic material. In iron alloys.

Occurrence Abundance in Earth's crust ~1 ppm. Occurs in small quantities in monazite, cerite and gadolinite.

Physical properties

M. Pt. 1356°C B. Pt. 3041°C Specific gravity 8.234 at 20°C

Environmental fate

Abiotic removal

Readily oxidised in air (1).

Genotoxicity

In vitro mouse JB6 epidermal cells induction of neoplastic transformations positive (2).

Other effects

Any other adverse effects

May impair blood coagulation (3).

Other comments

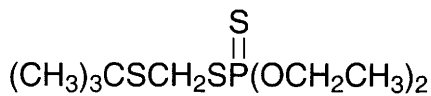
Terbium is a pharmacological analogue of calcium (2).

The kinetics of binding of terbium(III) to chicken ovotransferrin were studied (4).

References

1. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
2. Smith, B. M. et al *Carcinogenesis (London)* 1986, 7(12), 1949-1956.
3. Lewis, R. J. (Ed.) *Sax's Dangerous Properties of Industrial Materials* 8th ed., 1992, 3, 3190, Van Nostrand Reinhold, New York, NY, USA.
4. Teniguchi, T. et al *Eur. Biophys. J.* 1990, 18(1), 1-8

T22 terbufos



$\text{C}_9\text{H}_{21}\text{O}_2\text{PS}_3$

Mol. Wt. 288.44

CAS Registry No. 13071-79-9

Synonyms AC-92,100; Aragan; Counter; Contraven; Cyanater; *S*-*tert*-butylthiomethyl *O,O*-diethyl phosphorodithioate; *S*-[[[(1,1-dimethylethyl)thio]methyl] *O,O*-diethyl phosphorodithioate

EINECS No. 235-963-8

RTECS No. TD 7200000

Uses Insecticide. Nematicide.

Physical properties

M. Pt. -29.2°C **B. Pt.** 69°C at 0.01 mmHg **Flash point** 88°C (open cup) **Specific gravity** 1.105 at 24°C

Partition coefficient $\log P_{\text{ow}}$ 4.5185 (1) **Volatility** v.p. 2.6×10^{-4} mmHg at 25°C

Solubility Water: 4.5 mg l⁻¹ at 27°C. Organic solvents: acetone, benzene, chloroform, diethyl ether, ethanol, toluene

Occupational exposure

Supply classification very toxic

Risk phrases Very toxic in contact with skin and if swallowed (R27/28)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Wear suitable protective clothing and gloves - In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S36/37, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bluegill sunfish, rainbow trout 4, 10 µg l⁻¹, respectively (1).

Invertebrate toxicity

LD₅₀ topical bee 4.1 µg bee⁻¹ (2).

LC₅₀ (96 hr) juvenile red swamp crayfish *Procambarus clarkii* 5.9 µg l⁻¹. LC₅₀ (12 hr) dietary exposure 4.4 µg g⁻¹ pellet. Aberrant behaviour such as loss of motor control and equilibrium occurred at concentrations almost 50% of the aqueous LC₅₀ and 80% of the dietary LC₅₀ (3).

Environmental fate

Degradation studies

Undergoes oxidation and hydrolysis in soil with degradation t_{1/2} 4.5-27 days (1,4).

Adsorption and retention

Terbufos was immobile in sand, sandy loam, silt loam and silt clay soils (5).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse, dog, quail 1.6, 3.5, 4.5, 15 mg kg⁻¹, respectively (1,6-10).

LC₅₀ (4 hr) inhalation ♂, ♀ rat 1.2, 6.1 mg m⁻³, respectively (1).

LD₅₀ dermal rabbit, rat 1.0, 9.8 mg kg⁻¹, respectively (1,6,7).

Instillation of 0.1 mg into rabbit eyes was fatal to all animals within 2-24 hr (7).

Sub-acute and sub-chronic data

LC₅₀ (8 day) oral ring-necked pheasant, mallard duck 145, 185 mg kg⁻¹ diet, respectively (1).

Oral dog 0.05 mg kg⁻¹ day⁻¹ for 28 days inhibited plasma cholinesterase activity. Red blood cell cholinesterase activity was not inhibited by this dose (11).

Carcinogenicity and chronic effects

Oral rat (2 yr) 1 mg kg⁻¹ diet caused no adverse effects other than cholinesterase depression and associated syndrome (1).

Oral mouse 0, 0.45, 0.90 or 1.80 mg kg⁻¹ day⁻¹ for 18 months did not induce any carcinogenic effects (12).

Oral mouse 0, 0.075, 0.30 or 1.2 mg kg⁻¹ day⁻¹ for 18 months. Toxic effects noted were alopecia, signs of ataxia, exophthalmia in ♂ mice, corneal cloudiness and opacity, and eye rupture (13).

Teratogenicity and reproductive effects

Oral ♂, ♀ rats 0, 12.5 or 50 µg kg⁻¹ day⁻¹ for 60 days prior to mating. The high dose induced an increase in the frequency of litters with dead offspring (14).

Gavage rat 0.05, 0.10 or 0.20 mg kg⁻¹ day⁻¹ on days 6-15 of gestation. Slightly decreased maternal body weight was observed for the 0.10 and 0.20 mg kg⁻¹ doses. No foetotoxic or teratogenic effects were observed (15).

Gavage rabbit 0, 0.1, 0.2 or 0.4 mg kg⁻¹ day⁻¹ on days 7-19 of gestation. Maternal survival rates were 100%, 100%, 89% and 67%, respectively. The incidence of foetuses with an accessory left subclavian artery was significantly greater in the high-dose group. The incidence of an extra unilateral rib and of chain fusion of sternbrae was significantly lower in the high-dose group (16).

Metabolism and toxicokinetics

Readily absorbed following oral administration to mammals. Undergoes oxidation and hydrolysis. 50% of the dose to rats was eliminated in the urine within 15 hr. After 168 hr 83% had been eliminated in the urine and 3.5% in the faeces (species unspecified) (1,17).

Results from human exposure showed that dermal and inhalation absorption were negligible (18,19).

Irritancy

Irritating to the skin and eyes (species unspecified) (1).

Genotoxicity

In vitro Chinese hamster ovary cells, chromosomal aberrations with and without metabolic activation negative (20).

In vitro primary rat hepatocytes unscheduled DNA repair negative (21).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (22).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (23).

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th amendments) (24). WHO Toxicity Class Ia (25).

EPA Toxicity Class I (formulation) (2).

ADI (JMPR) 0.0002 mg kg⁻¹ body weight (25).

Other comments

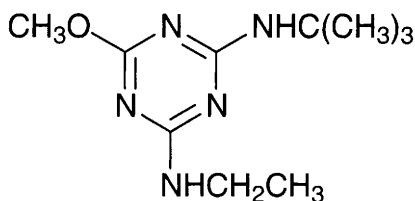
Residues have been detected in natural waters (4).

Physical properties, occurrence, environmental fate, metabolism, mammalian toxicity, teratogenicity, carcinogenicity, health advisories and analysis reviewed (4).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
3. Fornstrom, C. B. et al *Environ. Toxicol. Chem.* 1997, 16(12), 2514-2520.
4. *Drinking Water Health Advisories: Pesticides* 1989, 759-776, US EPA Office of Drinking Water Health Advisories, Lewis Publishers, Chelsea, MI, USA.
5. Jui, T. *Report* 1973, PD-M-108 455-483, MRID 87673, American Cyanamid Co. Princeton, NJ, USA.
6. *Farm Chemicals Handbook* 1983, C63, Meister Publishing, Willoughby, OH, USA.
7. *Report* 1972, Summary of Studies 093580-A through 093580-0, MRID 35960, American Cyanamid Co., Princeton, NJ, USA.
8. Consultox Laboratories *Acute Oral and Percutaneous Toxicity Evaluation* 1975, MRID 29863.
9. *Ecotox. Environ. Safety* 1984, 8, 551.
10. Parke, G. S. E. et al *Report* 1976, EPA File Symbol 2749-VEL, Laboratory No. 6E-3164, MRID 35121.
11. Berger, H. *Toxicology Report No. A A77-158* 1977, MRID 63189.
12. Tegeris Labs. Inc. *Chronic Dietary Toxicity and Oncogenicity Study with AC 92,100 (Terbufos) in Mice* 1986, EPA Accession No. 400986.
13. Rapp, R. A. et al *Report* 1974, Biodynamics Inc. Project No. 71R-728.
14. Smith, J. M. et al *Report* 1972, Project No. 71R-727, MRID 37473, American Cyanamid Co., Princeton, NJ, USA.
15. Rodweel, D. *Report* 1985, W.I.L. Research Laboratories Inc. Project No. WIL-35014, MRID 147553.
16. MacKenzie, K. *Report* 1984, Hazelton Laboratories America Inc. Study No. 6123-116, MRID 147532.
17. North, N. H. *Report* 1973, MRID 87695, American Cyanamid Co. Princeton, NJ, USA.
18. Peterson, R. G. et al *Farm Worker Study with Aerial Application of Counter 15-G* 1984, Report No. C-2370, MRID 137760.
19. Devine, J. M. et al *Arch. Environ. Contam. Toxicol.* 1985, 15(1), 113-122.
20. Thilager, A. et al *Chromosome Aberration in Chinese Hamster Ovary Cells* 1983, Microbiological Associate Study No. T1906 337006, MRID 133296.
21. Godek, E. R. et al *Rat Hepatocyte Primary Culture/DNA Repair Test* 1983, AC 92,100, PH311-AC-001-83, MRID 87693.
22. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
23. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
24. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
25. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21

T23 terbutumeton



C₁₀H₁₉N₅O

Mol. Wt. 225.29

CAS Registry No. 33693-04-8

Synonyms *N*²-*tert*-butyl-*N*⁴-ethyl-6-methoxy-1,3,5-triazine-2,4-diamine; *N*-(1,1-dimethylethyl)-*N'*-ethyl-6-methoxy-1,3,5-triazine-2,4-diamine; 2-methoxy-4-ethylamino-6-*tert*-butylamino-s-triazine

EINECS No. 251-637-9

Uses Herbicide for the selective control of grasses and broad-leaved weeds.

Physical properties

M. Pt. 123-124°C Specific gravity 1.08 at 20°C Partition coefficient log P_{ow} 3.04 Volatility v.p. 2.03 × 10⁻⁶ mmHg (20°C)

Solubility Water: 130 mg l⁻¹ at 20°C. Organic solvents: acetone, dichloromethane, methanol, *n*-octanol, toluene

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) rainbow trout, bluegill sunfish, crucian carp 14, 21, 30 mg l⁻¹, respectively (1).

Invertebrate toxicity

ED₅₀ (survival) *Tetrahymena pyriformis* 1.1 mg l⁻¹ (2).

LC₅₀ (48 hr) *Daphnia magna* 40 mg l⁻¹ (1).

Non-toxic to bees (1).

Environmental fate

Degradation studies

Undergoes microbial demethylation in soil to the hydroxytriazine. DT₅₀ in soil approximately 300 days (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 483 mg kg⁻¹ (3).

LD₅₀ oral mouse 2343 mg kg⁻¹ (1).

Inhalation LC₅₀ (4 hr) rat >10 mg l⁻¹ (1).

LD₅₀ dermal rat >3170 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

Oral rat (90 day) no-observed-effect level 10 mg kg⁻¹ day⁻¹ (1).

Oral dog (90 day) no-observed-effect level 25 mg kg⁻¹ day⁻¹ (1).

Metabolism and toxicokinetics

Rapidly absorbed following oral administration in mammals. More than 90% is eliminated within 24 hr, mainly in the urine, with around 25% in the faeces (1).

Irritancy

Non-irritating to skin of rats; slightly irritating to eyes of rabbits (1).

Legislation

WHO Toxicity Class II (4).

EPA Toxicity Class III (1).

Limited under EC Directive on Drinking Water Quality 80/788/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (5).

Included in Schedules 5 and 6 (Release into Water and Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (6).

ADI 0.075 mg kg^{-1} body weight (1).

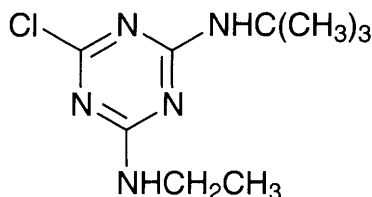
Other comments

Photosynthetic electron transport inhibitor (1).

References

1. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
2. Toth, D. et al *Biologia (Bratislava)* 1979, **34**(3), 233-239.
3. *Guide to the Chemicals Used in Crop Protection* 1973, Information Canada, 171 Slater St., Ottawa, Ontario, Canada.
4. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
5. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
6. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T24 terbutylazine



$\text{C}_9\text{H}_{16}\text{ClN}_5$

Mol. Wt. 229.71

CAS Registry No. 5915-41-3

Synonyms *N*²-*tert*-butyl-6-chloro-*N*⁴-ethyl-1,3,5-triazine-2,4-diamine; 6-chloro-*N*-(1,1-dimethylethyl)-*N*'-ethyl-1,3,5-triazine-2,4-diamine; 2-(*tert*-butylamino)-4-chloro-6-ethylamino-*s*-triazine

EINECS No. 227-637-9

RTECS No. XY 4550000

Uses Herbicide.

Physical properties

M. Pt. 177-179°C **Specific gravity** 1.188 at 20°C **Partition coefficient** $\log P_{ow}$ 3.21 (un-ionised)

Volatility v.p. 1.1×10^{-6} mmHg at 20°C

Solubility Water: 8.5 mg l^{-1} at 20°C. Organic solvents: dimethylformamide, ethyl acetate, isopropanol, octan-1-ol, tetraline, xylene

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) rainbow trout, goldfish $4.6\text{--}9.4 \text{ mg l}^{-1}$ (1).

LC₅₀ (96 hr) crucian carp, bluegill sunfish 52, 66 mg l^{-1} , respectively (1).

Invertebrate toxicity

EC₅₀ (48 hr) *Daphnia magna* >5 mg l⁻¹ (limited solubility) (2).

LD₅₀ (oral and contact) >100 µg bee⁻¹ (3).

Bioaccumulation

Calculated bioconcentration factor of 185 indicates that environmental accumulation would not be significant (4).

Environmental fate

Degradation studies

Undergoes microbial degradation in soil via dealkylation of the side chain, hydroxylation resulting from hydrolysis of the chlorine atoms and of the dealkylated amino group, and ring cleavage. t_{1/2} in soil 30-90 days (1).

Abiotic removal

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated t_{1/2} 3.0 hr (5).

Hydrolysis t_{1/2} 63 days at pH 5, >200 days at pH 7 and pH 9. Hydrolysis product is 2-hydroxy-4-*tert*-butylamino-6-ethylamino-1,3,5-triazine (6).

Adsorption and retention

Calculated K_{oc} of 1350 indicates that terbuthylazine will adsorb to some soils and sediments (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 2200 mg kg⁻¹ (1).

LC₅₀ (4 hr) inhalation rat >3500 mg m⁻³ (1).

LD₅₀ dermal rabbit >3000 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

Oral rat (90 day) no-adverse-effect level 3.5 mg kg⁻¹ day⁻¹ (1).

Metabolism and toxicokinetics

Following oral administration to mammals 80-84% is eliminated in the urine and faeces within 24 hr (1).

Irritancy

Slight skin irritant to rabbits; non-irritating to rabbit eyes (1).

Genotoxicity

Mouse bone marrow micronucleus test negative in ♂ and ♀ mice (7).

Legislation

EC maximum residue limit for grapes 0.1 ppm (1).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (8).

WHO Toxicity Class Table 5 (9).

EPA Toxicity Class III (formulation) (3).

ADI 0.0022 mg kg⁻¹ (3).

Other comments

Inhibits photosynthetic electron transport (3).

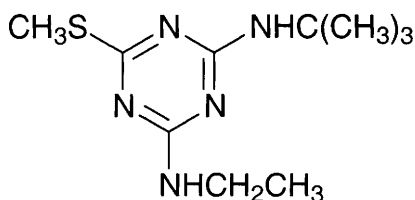
Metabolic pathways reviewed (10).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. Marchini, S. et al *Ecotoxicol. Environ. Saf.* 1988, **16**, 148-154.
3. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.

4. Kenagu, E. E. *Ecotoxicol. Environ. Saf.* 1980, **4**, 26-38.
5. Atkinson, R. et al *Int. Chem. Kinet.* 1987, **19**, 799-822.
6. Berkhard, N. et al *Pest. Sci.* 1981, **12**, 45-52.
7. Gebel, T. et al *Arch. Toxicol.* 1997, **71**(3), 193-197.
8. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
9. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
10. Roberts, T. R. et al (Eds.) *Metabolic Pathways of Agrochemicals. Part 1: Herbicides and Plant Growth Regulators* 1998, The Royal Society of Chemistry, Cambridge, UK

T25 terbutryn



C₁₀H₁₉N₅S

Mol. Wt. 241.36

CAS Registry No. 886-50-0

Synonyms Athado; *N*²-*tert*-butyl-*N*⁴-ethyl-6-methylthio-1,3,5-triazine-2,4-diamine; 2-(*tert*-butylamino)-4-(ethylamino)-6-methylthio-*s*-triazine; Clarosan; *N*-(1,1-dimethylethyl)-*N'*-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine; Plantonit; Igram; Prebane; Terbutrex

EINECS No. 212-950-5

RTECS No. XY 4725000

Uses Herbicide.

Physical properties

M. Pt. 104-105°C **B. Pt.** 154-160°C at 0.06 mmHg **Specific gravity** 1.115 at 20°C **Partition coefficient** log *P*_{ow} 3.65 at 25°C (un-ionised) (1) **Volatility** v.p. 9.1×10^{-7} mmHg at 20°C

Solubility Water: 22 mg l⁻¹ at 22°C. Organic solvents: acetone, carbon tetrachloride, chloroform, diethyl ether, dimethylformamide, dioxane, xylene

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bluegill sunfish, carp, perch, rainbow trout 3-4 mg l⁻¹ (1-3).

Invertebrate toxicity

EC₅₀ development of snail eggs, *Physa fontinalis* and *Lymaca stagnalis* 24 µg l⁻¹ (4).

LC₅₀ (48 hr) *Daphnia magna* 1.4-7.1 mg l⁻¹ (5,6).

Not toxic to bees. LD₅₀ (oral) >225 µg bee⁻¹ (7).

Bioaccumulation

Calculated bioconcentration factor is 100 (8).

Environmental fate

Degradation studies

Microbial degradation in soil *t*_{1/2} 14-20 days (1).

Abiotic removal

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated $t_{1/2}$ 3.1 hr (9).

Adsorption and retention

Calculated K_{oc} 700 (8).

Mammalian & avian toxicity**Acute data**

LD₅₀ oral rat, mouse 500, 3900 mg kg⁻¹, respectively (1,10).

LC₅₀ (4 hr) inhalation rat >8000 mg m⁻³ (1).

LD₅₀ dermal rat, rabbit >2000, >10,000 mg kg⁻¹, respectively (1).

LD₅₀ intraperitoneal rat, mouse 550, 700 mg kg⁻¹, respectively (10).

Sub-acute and sub-chronic data

LC₅₀ (8 day) oral bobwhite quail, mallard duck >20,000, >4600 mg kg⁻¹ diet, respectively (1).

Oral rat (90 day) no-adverse-effect level 50 mg kg⁻¹ day⁻¹ (1).

Oral dog (6 month) no-adverse-effect level 10 mg kg⁻¹ day⁻¹ (1).

Metabolism and toxicokinetics

Following oral administration to mammals 73-85% is eliminated as the dealkylated hydroxyl metabolite in the faeces (11).

Irritancy

Dermal rabbit 380 mg caused mild irritation and 76 mg instilled into rabbit eye caused moderate irritation (12).

Legislation

Approved for use in, or near, watercourses and lakes (5).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (13).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (14).

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th amendments) (15).

WHO Toxicity Class Table 5 (16).

EPA Toxicity Class III (formulation) (7).

ADI 0.027 mg kg⁻¹ (7).

Other comments

Metabolism in plants involves oxidation of the methylthio group to hydroxy metabolites, and dealkylation of the side chains (1).

Inhibits photosynthetic electron transport (7).

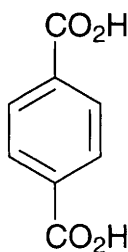
Metabolic pathways reviewed (17).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. *Handbook of Acute Toxicity of Chemicals to Fish and Aquatic Invertebrates* 1980, Resource Publ. No. 137, US Dept. Interior, Fish and Wildlife Service, Washington, DC, USA.
3. Toaby, T. E. et al *J. Fish Biol.* 1980, **16**(5), 521-597.
4. Kosanke, G. J. et al *Comp. Biochem. Physiol., C: Conf. Pharmacol. Toxicol.* 1988, **90C**, 373-379.
5. *Guidelines for the Use of Herbicides on Weeds in or near Watercourses and Lakes* 1985, Ministry of Agriculture, Fisheries and Food, Alnwick, UK.
6. Marchivi, S. et al *Ecotoxicol. Environ. Saf.* 1988, **16**, 148-157.
7. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
8. Keraga, E. E. *Ecotoxicol. Environ. Saf.* 1980, **4**, 26-38.
9. Atkinson, R. et al *Int. J. Chem. Kinet.* 1987, **19**, 799-828.
10. *Proc. Eur. Soc. Toxicology* 1976, **17**, 351.

11. Deng, K. et al *J. Agric. Food Chem.* 1990, **38**, 1411.
12. *Ciba-Geigy Toxicology Data* 1977, Ardsley, New York, NY, USA.
13. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
14. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
15. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; *6th Amendment EEC Directive* 79/831/EEC; *7th Amendment EEC Directive* 91/32/EEC 1991, HMSO, London, UK.
16. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
17. Roberts, T. R. et al (Eds.) *Metabolic Pathways of Agrochemicals. Part 1: Herbicides and Plant Growth Regulators* 1998, The Royal Society of Chemistry, Cambridge, UK

T26 terephthalic acid



C₈H₆O₄

Mol. Wt. 166.13

CAS Registry No. 100-21-0

Synonyms 1,4-benzenedicarboxylic acid; *p*-benzenedicarboxylic acid; *p*-phthalic acid; TA12; TA-33MP

EINECS No. 202-830-0

RTECS No. WZ 0875000

Uses In antiseptic formulation. Manufacture of polymers.

Occurrence Isolated from the pods of *Cassia roxburghii* and *Tephrosia hamiltonii*.

Physical properties

M. Pt. 300°C (sublimes) **Flash point** 260°C (open cup) **Specific gravity** 1.51 **Volatility** v.den. 5.74

Solubility Water: 16 mg l⁻¹. Organic solvents: ethanol

Occupational exposure

US-TWA 10 mg m⁻³

Ecotoxicity

Bioaccumulation

Estimated bioconcentration factor of 19 indicates that environmental accumulation is unlikely (1).

Environmental fate

Degradation studies

Degraded by soil microflora in 2 days (2).

Degraded under anaerobic conditions by the denitrifying bacterium *Pseudomonas* sp. strain P136 (3).

Catabolised by *Rhodococcus rubropertinctus* involving formation of benzoate, then 4-hydrobenzoate, protocatechinate, pyrocatechol and cyclic ortho-cleavage (4).

Abiotic removal

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated t_{1/2} 58 days (5).

Adsorption and retention

Estimated K_{oc} 292 indicates moderate adsorption to soils and sediments (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 10,000, 19,000 mg kg⁻¹, respectively (6,7).

LD₅₀ intraperitoneal mouse 1400 mg kg⁻¹ (8).

LD_{Lo} intravenous dog 770 mg kg⁻¹ (9).

Sub-acute and sub-chronic data

Inhalation rat (14 days) 0, 100, 200 or 400 mg m⁻³ for 30 min daily. There were no adverse changes in pulmonary function, bronchoalveolar lavage parameters, or evidence of histopathological changes. Reversible, dose-related rhinorrhoea and mild irritation of the mucous membranes were reported (10).

Carcinogenicity and chronic effects

Oral rat 20, 140 or 1000 mg kg⁻¹ diet for 2 yr. Body weight and food consumption were reduced, with decreased heart, lung, liver and kidney weight in high-dose ♂ rats. Mid- and high-dose ♀ rats had decreased heart and kidney weights and increased brain weights. The high dose induced bladder stones in ♀ rats, and histopathology revealed microconcentrations of calculi in the bladder. The incidence of bladder tumours in high-dose ♀ was 19/118, and of squamous metaplasia was 11/118 (11).

Teratogenicity and reproductive effects

Inhalation rat 0, 1, 5 or 10 mg m⁻³, 6 hr day⁻¹ on days 6-15 of gestation caused neither maternal or foetal toxicity nor any teratogenic effects (12).

Oral rat, one-generation study, 0, 0.03, 0.125, 0.5, 2.0 or 5% diet for 90 days throughout mating, gestation, lactation and post-weaning caused foetal and neonatal mortality in the two highest-dose groups. There was no effect on fertility index or litter size (13).

Metabolism and toxicokinetics

Rapidly excreted in the urine of rats following oral administration. No evidence of metabolism was observed.

Crosses the placenta in rats (14).

Irritancy

500 mg instilled into rabbit eye for 24 hr caused moderate irritation (7).

Inhalation rat (30 min) 400 mg m⁻³ caused mild irritation of the mucous membranes (10).

Sensitisation

Salmonella typhimurium TA98, TA100, TA1535, TA1538 with and without metabolic activation negative (15).

In vitro Chinese hamster ovary cells HGPRT assay and sister chromatid exchanges negative (15).

Other comments

Effects of terephthalic acid on the formation of bladder calculi and bladder cancer reviewed (16).

Toxicity and environmental impact reviewed (17).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (18).

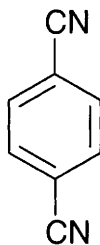
Autoignition temperature 496°C.

References

1. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behaviour of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
2. Alexander, M. et al *J. Agric. Food Chem.* 1966, **14**, 410.
3. Nozawa, T. et al *J. Bacteriol.* 1988, **170**(12), 5778-5784.
4. Naumova, R. P. et al *Mikrobiologiya* 1986, **55**(6), 918-923 (Russ.) (*Chem. Abstr.* **106**, 81380f).
5. Atkinson, R. *Int. J. Chem. Kinet.* 1987, **19**, 799-828.
6. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
7. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysvetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.

8. *Chem. Pharm. Bull.* 1968, **16**, 1655.
9. *Toxicol. Appl. Pharmacol.* 1971, **18**, 469.
10. Thomson, S. A. et al *Report* 1988, Chem. Res. Dev. Eng. Centre, Aberdeen Proving Ground, MD, USA.
11. ITT Research Institute *Chronic Dietary Administration of Terephthalic Acid* 1983, EPA Doc. No. FYI-OTS-0584-0190.
12. Ryan, B. M. et al *Toxicologist* 1990, **10**(1).
13. Research Triangle Institute *Ninety Day Study of Terephthalic Acid* 1982, EPA Doc. No. FYI-OTS-0482-0190.
14. Walowski-Tyl, R. et al *Drug Metabol. Dispos.* 1982, **10**(5), 486-490.
15. Brooks, A. L. et al *Environ. Mol. Mutagen.* 1989, **13**(4), 304-313.
16. D'Arcy Heck, H. *Banbury Rep.* 1987, **25**, 233-244.
17. *Dangerous Prop. Ind. Mater. Rep.* 1988, **8**(4), 68-71.
18. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T27 terephthalonitrile



$C_8H_4N_2$

Mol. Wt. 128.13

CAS Registry No. 623-26-7

Synonyms *p*-benzenenitrile; 4-cyanobenzonitrile; 1,4-dicyanobenzene; *p*-dicyanobenzene

EINECS No. 210-783-2

RTECS No. CZ 1925000

Uses Electron acceptor in photochemical reaction. Fluorescence quencher. Organic synthesis.

Physical properties

M. Pt. 224-227°C Volatility v.den. 4.42

Solubility Organic solvents: methanol

Ecotoxicity

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 70 ppm Microtox test (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 21,000 mg kg⁻¹ (2).

LD₅₀ intraperitoneal rat, mouse 700, 4000 mg kg⁻¹, respectively (3,4).

Irritancy

500 mg instilled into rabbit eye for 24 hr caused mild irritation (2).

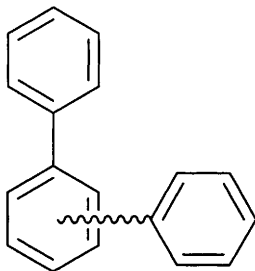
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (5).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
2. Marhold, J. V. *Sbornik Vysledku Toxilogickeho Vyetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
3. *Ind. Health* 1966, **4**, 11.
4. *Annals. Pharmaceut. Francais* 1990, **48**, 23.
5. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T28 terphenyl



C₁₈H₁₄

Mol. Wt. 230.31

CAS Registry No. 26140-60-3

Synonyms Delowax S; Delowax OM; diphenylbenzene; terbenzene

EINECS No. 247-477-3

RTECS No. WZ 6450000

Uses Solvent.

Occurrence In fossil fuels (1).

Physical properties

Solubility Organic solvents: benzene, diethyl ether, ethanol

Occupational exposure

FR-VLE 0.5 ppm (5 mg m⁻³)

UK-STEL 0.5 ppm (4.8 mg m⁻³)

US-STEL ceiling limit 5 mg m⁻³

Environmental fate

Nitrification inhibition

Not inhibitory to nitrification in activated sludge at 50 mg l⁻¹ (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 13,000 mg kg⁻¹ (3).

Sub-acute and sub-chronic data

Oral rat 33 mg kg⁻¹ day⁻¹ caused liver damage (duration unspecified) (4).

Inhalation rat 500 mg m⁻³, 7 hr day⁻¹ for 8 days caused morphological changes in mitochondria of pulmonary cells (4).

Sensitisation

Intracutaneous administration to guinea pigs caused sensitisation and necrosis (5).

Other effects

Other adverse effects (human)

Caused pulmonary irritation in exposed workers. No skin sensitisation was observed (4).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (6).

Other comments

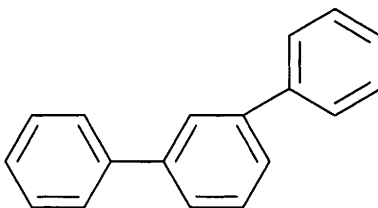
Identified in vehicle exhaust emissions and cigarettes smoke condensate (1).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (7).

References

1. Williams, R. et al *Int. J. Environ. Anal. Chem.* 1986, **26**(1), 27-49.
2. Wood, L. B. et al *Water Res.* 1981, **15**, 543-551.
3. *Shiyon Huagong* 1986, **15**, 305.
4. *Documentation of Threshold Limit Values* 4th ed., 1980, American Conference of Governmental Industrial Hygienists, Cincinnati, OH, USA.
5. Gosselin, R. E. et al *Clinical Toxicology of Commercial Products* 4th ed., 1976, **II**, 105, Williams and Wilkins, Baltimore, MD, USA.
6. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
7. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T29 *m*-terphenyl



C₁₈H₁₄

Mol. Wt. 230.31

CAS Registry No. 92-06-8

Synonyms *m*-diphenylbenzene; 1,3-diphenylbenzene; isodiphenylbenzene; 3-phenyldiphenyl; Santowax M; *m*-triphenyl; 1,3-terphenyl

EINECS No. 202-122-1

RTECS No. WZ 6470000

Uses Coolant in nuclear reactors. Solvent. In thermal printing material.

Physical properties

M. Pt. 86-87°C **B. Pt.** 379°C **Flash point** 191°C (open cup) **Specific gravity** 1.20

Solubility Organic solvents: acetic acid, benzene, diethyl ether, ethanol

Occupational exposure

UK-STEL 0.5 ppm (4.8 mg m⁻³)

US-STEL 0.53 ppm (5 mg m⁻³)

Environmental fate

Degradation studies

Converted into *p*-hydroxylated derivative by *Aspergillus parasiticus* (1).

Pseudomonas desmolyticum has been shown to grow on and degrade *m*-terphenyl (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 2400 mg kg⁻¹ (3).

Sub-acute and sub-chronic data

Oral rat 250-500 mg kg⁻¹ day⁻¹ for 30 days caused an increase in the liver:body weight ratio (4).

Metabolism and toxicokinetics

Major metabolites are glucosiduronic acids and free phenols (species unspecified) (5).

Irritancy

Irritating to the skin, eyes, mucous membranes and upper respiratory tract (species unspecified) (6).

Genotoxicity

Salmonella typhimurium TM677 with and without metabolic activation negative (7).

Other effects

Other adverse effects (human)

The only reported effects among exposed workers were reversible skin rashes (4).

Any other adverse effects

Inhalation exposure was reported to be fatal to laboratory animals, causing acute tracheal necrosis, tracheobronchitis, bronchopneumonia, atelectasis and petechial haemorrhages (5).

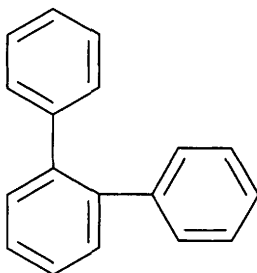
Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (8).

References

1. Salvo, J. J. et al *Biotechnol. Prog.* 1990, **6**(3), 193-197.
2. Catelai, D. et al *Experientia* 1970, **26**(8), 922.
3. Cornish, H. H. et al *Am. Ind. Hyg. Assoc. J.* 1962, **23**, 372.
4. Weeks, J. L. et al *J. Occup. Med.* 1970, **12**(7), 246.
5. Gosselin, R. E. et al *Clinical Toxicology of Commercial Products* 4th ed., 1976, **II**, 105, Williams & Wilkins, Baltimore, MD, USA.
6. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3223, Sigma-Aldrich, Milwaukee, WI, USA.
7. Kader, D. A. et al *Cancer Res.* 1979, **39**, 4152.
8. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T30 o-terphenyl



C₁₈H₁₄

Mol. Wt. 230.31

CAS Registry No. 84-15-1

Synonyms 1,2-diphenylbenzene; 1,1':2',1''-terphenyl; 2-phenylbiphenyl

EINECS No. 201-517-6

RTECS No. WZ 6472000

Uses Solvent.

Physical properties

M. Pt. 58-59°C **B. Pt.** 337°C **Flash point** 110°C (99% purity) **Volatility** v.p. 1.1×10^{-2} mmHg at 70°C; v.den. 7.95

Solubility Organic solvents: acetone, benzene, chloroform, ethanol, methanol

Occupational exposure

UK-STEL 0.5 ppm (4.8 mg m⁻³)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1900 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

Oral rat (30 day) 250 or 500 mg kg⁻¹ body weight day⁻¹ caused an increase in liver and kidney weight ratios (2).

Metabolism and toxicokinetics

Following intragastric administration of 80 mg kg⁻¹, ¹⁴C-labelled substance to rats, ~10% of radioactivity in the faeces during the first 24 hr was found as unmetabolised 1,2-diphenylbenzene, ~86% as free phenols, and the remaining 4% as non-hydrolysed, conjugated polar metabolites. When administered to rabbits, 12% of radioactivity in urine during the first 24 hr was found as unmetabolised substance, 79% as free phenols, and the remaining 9% as conjugated polar metabolites (3).

Irritancy

Irritating to the eyes, skin, mucous membranes and upper respiratory tract (species unspecified) (4).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (5).

Other comments

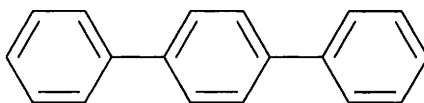
Residues have been isolated from river water and sediments (6).

References

1. Cornish, H. H. et al *Am. Ind. Hyg. Assoc. J.* 1962, 23, 372.

2. *Documentation of Threshold Limit Values* 4th ed., 1980, 388, American Conference of Governmental Industrial Hygienists, Cincinnati, OH, USA.
3. Scoppa, P. et al *Boll. Soc. Ital. Biol. Sper.* 1971, **47**(7), 194.
4. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, 2, 3223.
5. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
6. Yamashita, K. et al *Kagoshima-Ken Kankyo Senta Shoho* 1988, **4**, 88-95 (Japan.) (*Chem. Abstr.* **112**, 240098n)

T31 *p*-terphenyl



$C_{18}H_{14}$

Mol. Wt. 230.31

CAS Registry No. 92-94-4

Synonyms *p*-diphenylbenzene; 1,4-diphenylbenzene; 4-phenylbiphenyl; Santowax P; *p*-triphenyl; 1,1':4',1''-terphenyl

EINECS No. 202-205-2

RTECS No. WZ 6475000

Uses Laser dye. Solvent.

Occurrence Occurs in petroleum oil.

Physical properties

M. Pt. 212-213°C **B. Pt.** 389°C **Flash point** >110°C (open cup) **Specific gravity** 1.234 at 0°C with respect to water at 4°C **Partition coefficient** $\log P_{ow}$ 6.03

Solubility Organic solvents: benzene, ethanol

Occupational exposure

UK-STEL 0.5 ppm (4.8 mg m⁻³)

US-STEL ceiling limit 0.53 ppm (5 mg m⁻³)

Mammalian & avian toxicity

Acute data

LD_{Lo} oral rat 500 mg kg⁻¹ (1).

LD₅₀ oral rat >10,000 mg kg⁻¹ (2).

Sub-acute and sub-chronic data

Oral rat 2500-5000 mg kg⁻¹ day⁻¹ for 1 month affected liver function and caused an insignificant decrease in body weight (target organs not specified) (3).

Inhalation rat 35 mg m⁻³ for 1 month caused functional and morphological changes (3).

Inhalation rat 2000 mg m⁻³, 4 hr day⁻¹, 5 days wk⁻¹ for 8 wk produced cell debris in the lungs which rapidly cleared on termination of exposure (4).

Irritancy

Irritating to the skin, eyes, mucous membranes and upper respiratory tract (species unspecified) (5).

Legislation

The $\log P_{ow}$ value exceeds the European Community recommended level of 3.0 (Directive on Classification, Packaging and Labelling Dangerous Substances, 6th and 7th Amendments) (6).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (7).

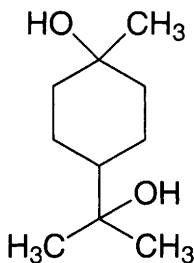
Other comments

Residues have been identified in river sediments and in emissions from vehicle exhausts (8,9).
Autoignition temperature 535°C.

References

1. National Academy of Sciences Report 1953, 5, 26, NRC, Chemical-Biological Coordination Center, Washington, DC, USA.
2. Cornish, H. H. et al *Am. Ind. Hyg. Assoc. J.* 1962, 23, 372.
3. Khromerko, Z. F. *Nauch. Tr. Inkutsk. Med. Inst.* 1972, 115, 121.
4. Adamson, I. Y. R. *Arch. Environ. Health* 1973, 26(4), 192.
5. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, 2, 3223.
6. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
7. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
8. Yamashita, K. et al *Kagoshima-Ken Kankyo Senta Shoho* 1988, 4, 88-95 (Japan.) (*Chem. Abstr.* 112, 240098n).
9. Williams, R. et al *Int. J. Environ. Anal. Chem.* 1986, 26(1), 27-49

T32 terpin



$C_{10}H_{20}O_2$

Mol. Wt. 172.27

CAS Registry No. 80-53-5

Synonyms 4-hydroxy- $\alpha,\alpha,4$ -trimethylcyclohexanemethanol; dipentane glycol; *p*-menthane-1,8-diol; 1,8-terpin

EINECS No. 201-288-2

Uses Manufacture of disinfectants; *cis*-form (hydrate) used as expectorant.

Occurrence In eucalyptus leaf oil.

Physical properties

M. Pt. 154-159°C

Solubility Organic solvents: vegetable oils

Ecotoxicity

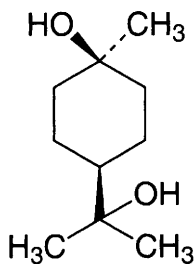
Fish toxicity

Not toxic to brown trout, bluegill sunfish, yellow perch and goldfish exposed to 5 ppm for 24 hr. Test conditions: pH 7; dissolved oxygen 7.5 ppm; total hardness (soap method) 300 ppm; methyl orange alkalinity 310 ppm; free carbon dioxide 5 ppm; and 12.8°C (1).

References

1. Wood, E. M. *The Toxicity of 3400 Chemicals to Fish* 1987, EPA560/6-87-002; PB87-200-275, Washington, DC, USA

T33 *cis*-1,8-terpin



$C_{10}H_{20}O_2$

Mol. Wt. 172.27

CAS Registry No. 565-48-0

Synonyms *cis*-*p*-menthane-1,8-diol; (1*RS*,4*RS*)-*p*-menthane-1,8-diol

EINECS No. 209-279-5

Uses Expectorant.

Occurrence Isolated from the leaves of *Cupressus torulosa* and the fruit of *Schinus molle*.

Physical properties

M. Pt. 104-105°C **B. Pt.** 258°C

Solubility Water: boiling water. Organic solvents: glacial acetic acid, chloroform, diethyl ether, ethanol, ethyl acetate, methanol, vegetable oils

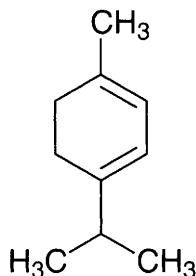
Other comments

Rapidly forms hydrate on exposure to air (1).

References

1. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA

T34 α -terpinene



C₁₀H₁₆

Mol. Wt. 136.24

CAS Registry No. 99-86-5

Synonyms FEMA No. 3558; 1-isopropyl-4-methyl-1,3-cyclohexadiene; *p*-mentha-1,3-diene; 1-methyl-4-isopropyl-1,3-cyclohexadiene; 1-methyl-4-(1-methylethyl)-1,3-cyclohexadiene

EINECS No. 202-795-1

RTECS No. OS 8060000

Uses Organic synthesis.

Occurrence In plant oils. Defensive secretion of termites.

Physical properties

B. Pt. 173-175°C **Flash point** 46°C **Specific gravity** 0.834 at 20°C with respect to water at 4°C

Solubility Water: practically insoluble. Organic solvents: diethyl ether, ethanol, fixed oils

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1700 mg kg⁻¹ (1).

Teratogenicity and reproductive effects

Oral ♀ Wistar rats 0, 30, 60, 125 or 250 mg kg⁻¹ body wt. by gavage in corn oil on days 6-15 of pregnancy. The two highest doses were maternally toxic. No increase in the ratio of resorptions/implantations was observed. A decrease in foetal body wt. and an increase in foetal kidney wt. occurred at the 250 mg kg⁻¹ level. There were signs of delayed ossification and minor skeletal malformations at doses of 60 mg kg⁻¹ or more. The no-observed-effect level for α -terpinene-induced embryofoetotoxicity was 30 mg kg⁻¹ by the oral route (2).

Irritancy

Irritating to the skin. Vapour or mist is irritating to the eyes, mucous membranes and upper respiratory tract (species unspecified) (3).

References

1. *Food Cosmet. Toxicol.* 1976, **14**, 873.
2. Araujo, I. B. et al *Food Chem. Toxicol.* 1996, **34**(5), 477-482.
3. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3223, Sigma-Aldrich, Milwaukee, WI, USA

T35 terpineol

$C_{10}H_{18}O$

Mol. Wt. 154.25

CAS Registry No. 8000-41-7

Synonyms FEMA No. 3045; *p*-menth-1-en-8-ol; mixture of *p*-methenols; Terpineol 318; terpinol

EINECS No. 232-268-1

RTECS No. WZ 6600000

Uses Binding agent for brazing pastes. Solvent. Fragrance. Antiseptic.

Occurrence In plant oils. Mixture of α , β and γ -isomers.

Physical properties

B. Pt. 214-225°C Flash point 91°C Specific gravity 0.930-0.936

Solubility Organic solvents: diethyl ether, ethanol, glycerol, vegetable oils

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 4300 mg kg⁻¹ (1).

LD₅₀ subcutaneous mouse 1400 mg kg⁻¹ (2).

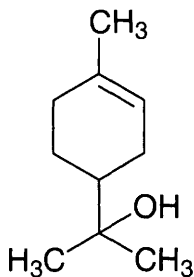
Irritancy

Dermal rabbit (24 hr) 500 mg caused moderate irritation (1).

References

1. *Food Cosmet. Toxicol.* 1974, 12, 807.
2. *Sapporo Igaku Zasshi* 1952, 3, 73

T36 α -terpineol



$C_{10}H_{18}O$

Mol. Wt. 154.25

CAS Registry No. 10482-56-1

Synonyms *p*-menth-1-en-8-ol; terpineol schlechthin; $\alpha,\alpha,4$ -trimethyl-3-cyclohexene-1-methanol

EINECS No. 202-680-6

RTECS No. WZ 6700000

Uses In perfumes. In denaturing of fats for soap manufacture. Antioxidant. Antiseptic. Fumigant. Solvent.

Occurrence In plant oils. Identified in tobacco smoke (1).

Physical properties

M. Pt. 31-35°C **B. Pt.** 217-218°C **Flash point** 89°C **Specific gravity** 0.935 at 20°C with respect to water at 20°C **Volatility** v.p. 0.023 mmHg at 20°C
Solubility Water: 2 g l⁻¹ at 20°C. Organic solvents: benzene, diethyl ether, ethanol, propylene glycol

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) rainbow trout 10-100 mg l⁻¹ at 10°C static bioassay (2).

Bioaccumulation

Estimated bioconcentration factor is 8.5-53 (3).

Environmental fate

Degradation studies

No biodegradation after 23 days under anaerobic conditions at an initial concentration of 4000 mg l⁻¹ (4).
99% removal when incubated under aerobic conditions for 168-192 hr using sewage inoculum in batch and continuous digesters (5).

Abiotic removal

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated t_{1/2} 4 hr (6).
Volatilisation t_{1/2} 19 days in model river water, 298 days in model pond water (3,4,7,8).

Adsorption and retention

Estimated K_{oc} of 67 indicates that adsorption to soil and sediments would not be significant (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 5200, 12,000 mg kg⁻¹, respectively (8,9).
LD₅₀ intramuscular mouse 2000 mg kg⁻¹ (10).

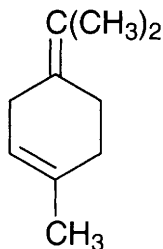
Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (11).

References

1. Florin, I. et al *Toxicology* 1980, **18**(3), 219.
2. GEMS: *Graphical Exposure Modeling System* 1982, US EPA, Washington, DC, USA.
3. Webb, M. et al *Water Res.* 1976, **10**, 303.
4. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
5. Hrutfiord, B. F. et al *Tappi* 1975, **58**, 98-100.
6. Francis, A. J. in *IAEA-SM-257/72 Environmental Migration of Long-Lived Radionuclides* 1982, International Atomic Energy Agency, Vienna, Austria.
7. Atkinson, R. *Int. J. Chem. Kinet.* 1987, **19**, 799-828.
8. EXAMS II *Computer Simulation* 1987, US EPA, Athens, GA, USA.
9. *Gig. Tr. Prof. Zabol.* 1987, **31**(2), 29.
10. *Zhongcaoyao* 1982, **13**, 241.
11. *J. Sci. Ind. Res. Sect. C: Biol. Sci.* 1962, **21**, 342

T37 terpinolene



C₁₀H₁₆

Mol. Wt. 136.24

CAS Registry No. 586-62-9

Synonyms 4-isopropylidene-1-methylcyclohexene; 1-methyl-4-isopropylidene-1-cyclohexene; 1-methyl-4-(1-methylethylidene)cyclohexene; *p*-mentha-1,4(8)-diene; 1,4(8)-terpadiene

EINECS No. 209-578-0

RTECS No. WZ 6870000

Uses In perfumes. Solvent for resins.

Occurrence In plant oils.

Physical properties

B. Pt. 185°C **Flash point** 38°C (closed cup) **Specific gravity** 0.8623 at 20°C with respect to water at 4°C

Partition coefficient log *P*_{ow} 4.23 (calculated) (1) **Volatility** v.p. 0.595 mmHg at 25°C

Solubility Water: 1.74 mg l⁻¹. Organic solvents: benzene, diethyl ether, ethanol, vegetable oils

Occupational exposure

UN No. 2541 **HAZCHEM Code** 3W **Conveyance classification** flammable liquid

Ecotoxicity

Bioaccumulation

Estimated bioconcentration factor of 966 indicates that environmental accumulation may occur (2).

Environmental fate

Abiotic removal

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated *t*_{1/2} 1.4 hr, and with ozone 1.7-23 min (3,4).

Volatilisation *t*_{1/2} 3.4 hr at 25°C in model river water, 41 days in model pond water (2,5).

Adsorption and retention

Calculated *K*_{oc} of 4766 indicates that adsorption to soil and sediments would be significant (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 4400 mg kg⁻¹ (6).

Irritancy

Not irritating to human or rabbit skin (7).

Sensitisation

Produced no sensitisation in human skin patch tests (7).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (8).
The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th Amendments) (9).

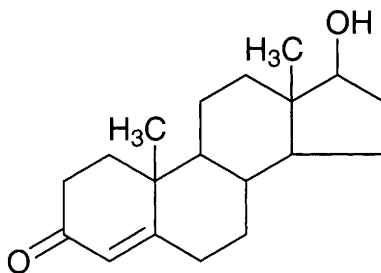
Other comments

Environmental fate reviewed (10).
Mixture of *p*-mentha-1,4(8)-diene and *p*-mentha-2,4(8)-diene

References

1. GEMS: Graphical Exposure Modeling System 1988, US EPA, Washington, DC, USA.
2. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
3. Atkinson, R. et al *Chem. Rev.* 1984, **84**, 437-470.
4. Atkinson, R. et al *Environ. Sci. Technol.* 1985, **19**, 159-163.
5. EXAMS II Computer Simulation 1987, US EPA, Athens, GA, USA.
6. *Food Cosmet. Toxicol.* 1986, **14**, 877.
7. Opdyke, D. L. J. (Ed.) *Monographs on Fragrance Raw Materials* 1979, 697, Pergamon Press, New York, NY, USA.
8. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
9. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
10. Howard, P. H. et al *Handbook of Environmental Fate and Exposure Data* 1993, **4**, 518-526, Lewis Publishers, Chelsea, MI, USA

T38 testosterone



$C_{19}H_{28}O_2$

Mol. Wt. 288.43

CAS Registry No. 58-22-0

Synonyms androlin; androst-4-en-17 β -ol-3-one; androsol; cristerone T; homosterone; 17 β -hydroxy- Δ^4 -androst-3-one; 17 β -hydroxyandrost-4-en-3-one; malestrone; neo-testis; promoteston; testandrone; testosterone hydrate; testoviron; virosterone; *trans*-testosterone

EINECS No. 200-370-5

RTECS No. XA 3030000

Uses Therapeutic androgen used in the treatment of hypogonadism, eunuchoidism and impotence in men. In women it is used for the treatment of metastatic breast cancer, post-partum breast engorgement and vasomotor symptoms of the climacteric.

Occurrence Naturally occurring σ^4 hormone secreted in mammalian testes (1).

Physical properties

M. Pt. 153-155°C

Solubility Organic solvents: acetone, chloroform, diethyl ether, 1,4-dioxane, ethanol, fixed oils

Mammalian & avian toxicity

Acute data

LD_{Lo} intraperitoneal rat 330 mg kg⁻¹ (2).

Sub-acute and sub-chronic data

Subcutaneous ♀ mouse (90 day) 100 µg animal⁻¹ day⁻¹ for first 10 days of life. The mice were ovariectomised at 60 days and killed at 90 days. In all mice, the cranial part of the vagina became lined with stratified epithelium, with either cornification, parakeratosis or mucification (3).

Carcinogenicity and chronic effects

Oral neonatal ♀ mouse 25 µg animal⁻¹ day⁻¹ for first 5 days after birth. 7/9 animals developed hyperplastic epithelial lesions, resembling epidermoid carcinomas (vaginal squamous-cell tumours), at ~71 wk of age (4). Subcutaneous neonatal ♀ mouse (16 month) 5 or 20 µg animal⁻¹ day⁻¹ for first 5 days of life resulted in mammary tumour incidences of 42/49 and 22/35, respectively, compared with 8/35 and 32/64 in oestradiol-17β treated mice, and 9/43 in vehicle controls (5).

The incidence of urinary bladder tumours in ♀ rats given 0.05% *N*-butyl-*N*-(4-hydroxybutyl)nitrosoamine in drinking water for 6 wk was not significantly altered by ovariectomy when compared with controls during 24 wk of observation (3/10 *vs.* 2/11). Subcutaneous implantation of 50 mg rat⁻¹ in the nitrosamine-treated ovariectomised rats increased the incidence of bladder tumours to 8/11. Testosterone treatment alone induced no tumours (6).

Teratogenicity and reproductive effects

Intramuscular rat, lowest toxic dose 8 mg kg⁻¹ day⁻¹ on days 13-20 of gestation (teratogenic effects) (7).

Intramuscular rat, lowest toxic dose 60 mg kg⁻¹ day⁻¹ on days 3-7 of gestation (pre-implantation mortality) (8).

Foetal virilisation following administration of testosterone to women during pregnancy has been reported (9).

Metabolism and toxicokinetics

Transformed to 5α-dehydrotestosterone in mammalian target organs such as the prostate, sebaceous glands and seminal vesicles (10).

Radioactivity from tritiated testosterone injected intravenously to rats was incorporated into the thymus gland, liver, prostate and muscle (11).

Readily absorbed from gastro-intestinal tract, skin and oral mucosa. It is largely metabolised to weakly androgenic endrosterone and inactive etiocholanolone, which are excreted in the urine mainly as glucuronides and sulfates. ~6% is excreted unchanged in the faeces. Testosterone absorbed from the gastro-intestinal tract is almost completely metabolised in the liver before it reaches the systemic circulation. Testosterone is extensively bound to a plasma globulin which also binds oestradiol. A small proportion is converted into oestrogenic derivatives. Only ~2% is unbound and the plasma *t*_{1/2} ranges from 10-100 minutes. Testosterone is believed to be converted into the more active dihydrotestosterone in some target organs (12).

Genotoxicity

Inhibited DNA synthesis in rat hepatocytes *in vitro* (13).

Other effects

Other adverse effects (human)

Reports of malignant neoplasms occurring in association with testosterone therapy have included carcinoma of the liver, prostatic cancer and renal cell carcinoma (12).

Side effects include an increase in the retention of nitrogen, sodium and water, oedema, increased vascularity of the skin, hypercalcaemia, impaired glucose tolerance, increased bone growth and skeletal weight. Other effects include increased low-density-lipoprotein cholesterol, decreased high-density-lipoprotein cholesterol, increased haematocrit and increased fibronolytic activity with increased risk of heart disease (12,14).

In ♂ large doses suppress spermatogenesis and cause degenerative changes in the seminiferous tubules (12).
In ♀ the inhibitory action on the activity of the anterior pituitary results in suppression of ovarian activity and menstruation. Continued administration of large doses produces symptoms of virilism (12).
Severe priapism was reported following administration for the management of delayed ♂ puberty (15).

Any other adverse effects

Various reports are cited on the masculinising effect of testosterone and testosterone propionate on ♀ mammalian foetuses (1).

Other comments

Physical properties, use, occurrence, analysis, carcinogenicity, mammalian toxicity and metabolism of testosterone and its ester reviewed (1).

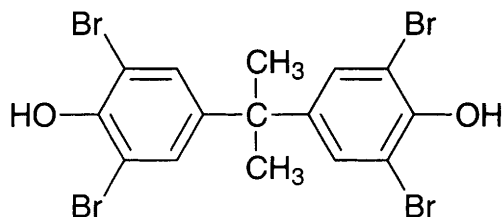
Subcutaneous implant mouse, 18 mg pellet significantly inhibited transformation of transplanted mammary tumour cells (16).

Sex hormones and Sjogren's syndrome reviewed (17).

References

1. IARC Monograph 1979, **21**, 519-547.
2. *Proc. Soc. Exp. Med.* 1941, **46**, 116.
3. Iguchi, T. et al *Endocrinol. Jpn.* 1976, **23**, 327-332.
4. Takasugi, N. et al in Kazda, S. et al (Eds.) *The Post-Natal Development of Phenotype* 1970, 229-251, Academia, Prague, Czechoslovakia.
5. Mori, T. et al *J. Natl. Cancer Inst.* 1976, **57**, 1057-1062.
6. Okayima, E. et al *Urol. Res.* 1975, **3**, 73-79.
7. *Endocrinology (Baltimore)* 1976, **99**, 1490.
8. *Endocrinology (Baltimore)* 1977, **100**, 1684.
9. Reschini, E. et al *Lancet* 1985, **i**, 1226.
10. Kochakian, C. D. (Ed.) *Handbook of Experimental Pharmacology* 1976, **43**, 287-359, Springer, Berlin, Germany.
11. Chermnykk, N. S. et al *Byoll. Cksp. Biol. Med.* 1988, **106**(11), 611-613 (Russ.) (*Chem. Abstr.* **110**, 33911r).
12. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
13. Nouicki, D. L. *Cancer Res* 1985, **45**, 337-344.
14. Glazer, G. *Arch. Inter. Med.* 1991, **151**, 1925-1933.
15. Ruch, W. et al *Am. J. Med.* 1989, **86**, 256.
16. Medina, D. et al *J. Natl. Cancer Inst.* 1977, **58**, 1107-1110.
17. Sullivan, D. A. *J. Rheumatol., Suppl.* 1997 1997, **50**, 17-32

T39 tetrabromobisphenol A



$C_{15}H_{12}Br_4O_2$

Mol. Wt. 543.88

CAS Registry No. 79-94-7

Synonyms 4,4'-isopropylidenebis(2,6-dibromophenol); 4,4'-(1-methylethylidene)bis(2,6-dibromophenol); 2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol; 2,2-bis(3,5-dibromo-4-hydroxyphenyl)propane; tetrabromodihydroxydiphenylpropane; TBBA; TBBPA

EINECS No. 201-236-9

Uses Reactive or additive flame retardant in polymers.

Physical properties

M. Pt. 181-182°C B. Pt. ~316°C Specific gravity 2.2 at 4°C Partition coefficient $\log P_{ow}$ 4.5-5.3

Volatility v.p. <1 mmHg at 20°C

Solubility Water: insoluble (<0.1 wt% at 25°C). Organic solvents: acetone, methanol

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr, flow-through) fathead minnow 0.54 mg l⁻¹, no-observed-effect concentration 0.26 mg l⁻¹ (1).

LC₅₀ (96 hr) *Brachydanio rerio* 2.9 µg l⁻¹ (2).

Invertebrate toxicity

LC₅₀ (48 hr) *Daphnia magna* 1.5 µg l⁻¹ (2).

LC₅₀ (96 hr) *Mysidopsis bahia* 800-1200 µg l⁻¹. The differences between age groups 1-5, 5-9, and 10-14 days were <2-fold (3).

EC₅₀ (72 hr) *Skeletonema costatum*, *Thalassiosira pseudonana* between 90-890 µg l⁻¹ and 130-1000 µg l⁻¹, respectively (4).

Environmental fate

Degradation studies

After 64 days under aerobic conditions 82% of the applied sample remained in soil composed of sand (83%), silt (13%) and clay (4%), and 36% remained in soil composed of sand (43%), silt (24%) and clay (33%). The corresponding values in these soils under anaerobic conditions were 43.7-57.4% and 53.4-65%, respectively. In soil composed of sand (16%), silt (58%) and clay (26%) under anaerobic conditions, 89.5-90.6% of the applied sample remained after 64 days (5).

No biodegradation could be detected using BOD for TBBA (100 mg l⁻¹) in sludge (30 mg l⁻¹) in a 2-wk study under sewage-treatment conditions (5).

Abiotic removal

Sterile soil t_{1/2} 1300 days (5).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat >3.2 and >2 g kg⁻¹ body weight, respectively (6).

A single oral or peritoneal dose of 500-1000 mg kg⁻¹ increased the level of malondialdehyde (an indicator of lipid peroxidation) in the liver (7).

Sub-acute and sub-chronic data

Oral rats 7 doses of 1100 mg kg⁻¹ (timing of doses unspecified) caused a 2-3-fold elevation of the level of malondialdehyde in the liver and caused steatosis. Increased GPT activity was observed after 3 doses (7). Gavage 6-7 wk old Sprague-Dawley rats (4 wk) 10-1000 mg kg⁻¹ day⁻¹. Threshold for decrease of body weight 0.3-3.0 mg kg⁻¹ day⁻¹. Weight ratio of kidney to body weight increased from 10 mg kg⁻¹ day⁻¹. The haematocrit value and clotting time decreased, and the cholesterol concentration, blood urea nitrogen concentration and choline esterase activity increased with all doses (8).

Teratogenicity and reproductive effects

♀ Rats treated with 0-2.5 g kg⁻¹ on days 0-19 of gestation. No impairment of the birth rate was observed and no toxic effects on embryos or foetuses. Postnatal development was not impaired (9).

Metabolism and toxicokinetics

Poorly absorbed from the rat gastro-intestinal tract, but then distributed throughout most of the organs of the body. Maximum t₅₀ in any rat tissue <2.5 days (5).

Irritancy

Not a skin irritant in 54 volunteers (5).

Not irritating to eyes of rabbit (5).

Sensitisation

Did not produce skin sensitisation in 54 volunteers (5).

Genotoxicity

Salmonella typhimurium TA100, TA1535, TA1537, TA98 with and without metabolic activation negative (10).

Other effects

Other adverse effects (human)

Stimulated proliferation of human breast cancer cells (MCF-7) but the oestrogenic potency was 4-6 orders of magnitude lower than 17β-oestradiol. Co-treatment with 5 × 10⁻⁶M tamoxifen antagonised the proliferative effect (11).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) of Statutory Instrument No. 472, 1991 (12).

Other comments

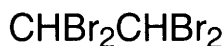
Dissolved humic material has no effect on the 24 and 48 hr LD₅₀s of tetrabromobisphenol A to *Daphnia magna* (13,2).

References

1. Surprenant, D. C. *Report No. 89-2-2937*, Springborn Life Sciences, Inc., Wareham, MA, USA.
2. Lee, S. K. et al *Water Res.* 1993, **27**(2), 199-204.
3. Goodman, L. R. et al *Bull. Environ. Contam. Toxicol.* 1988, **41**(5), 746-753.
4. Walsh, G. E. et al *Ecotoxicol. Environ. Saf.* 1987, **14**, 215-222.
5. *Environmental Health Criteria No. 172: Tetrabromobisphenol A and Derivatives*, 1995, WHO/IPCS, Geneva, Switzerland.
6. Gustafsson, K. et al *Status Report on Tetrabromobisphenol A* 1988, National Chemicals Inspectorate (Unpublished Report), Solna, Sweden.
7. Szymanska, J. A. *Ind. Chem. Libr.* 1995, **7**, 387-398.
8. Sato, T. et al *Toxicol. Environ. Chem.* 1996, **55**, 159-171.
9. Noda, T. *Annu. Rep. Osaka City Inst. Public Health Environ. Sci.* 1985, **48**, 106-121.
10. Mortelmans, K. et al *Environ. Mutagen.* 1986, **8**(Suppl. 7), 1-119.

11. Korner, W. et al *Organohalogen Compd.* 1996, **27**, 297-302.
12. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
13. Steinberg, C. E. W. et al *Acta Hydrochim. Hydrobiol.* 1992, **20**(6), 326-332

T40 1,1,2,2-tetrabromoethane



$\text{C}_2\text{H}_2\text{Br}_4$

Mol. Wt. 345.65

CAS Registry No. 79-27-6

Synonyms acetylene tetrabromide; Muthmann's liquid; TBE; *sym*-tetrabromoethane

EINECS No. 201-191-5

RTECS No. KI 8225000

Uses Solvent. Mercury substitute in gauges and balances. Refractive index liquid in microscopy. Separates metals by density.

Physical properties

M. Pt. -1 to 1°C **B. Pt.** 119°C at 15 mmHg **Specific gravity** 2.9638 at 20°C with respect to water at 4°C

Volatility v.p. <0.1 mmHg at 20°C; v.den. 11.9

Solubility Water: 6.5 mg l⁻¹ at 30°C. Organic solvents: acetone, aniline, glacial acetic acid, chloroform, diethyl ether, ethanol

Occupational exposure

DE-MAK 1 ppm (14 mg m⁻³)

FR-VME 1 ppm (15 mg m⁻³)

SE-LEVL 1 ppm (14 mg m⁻³)

SE-STEL 2 ppm (30 mg m⁻³)

UK-LTEL 0.5 ppm (7.2 mg m⁻³)

US-TWA 1 ppm (14 mg m⁻³)

UN No. 2504 **HAZCHEM Code** 2☒ **Conveyance classification** toxic substance

Supply classification very toxic

Risk phrases Very toxic by inhalation – Irritating to the eyes – Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R26, R36, R52/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Avoid contact with the skin – Take off immediately all contaminated clothing – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S24, S27, S45, S61)

Ecotoxicity

Bioaccumulation

Calculated bioconcentration factor of 97 indicates that environmental accumulation would not be significant (1).

Environmental fate

Abiotic removal

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated t_{1/2} 1.8 months (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, guinea pig, rabbit, rat 270, 400, 400, 1200 mg kg⁻¹, respectively (3-6).

LC₅₀ (4 hr) inhalation rat 550 mg m⁻³ (6).

LD₅₀ dermal rat 5250 mg kg⁻¹ (6).

LD₅₀ intraperitoneal mouse 440 mg kg⁻¹ (7).

Sub-acute and sub-chronic data

Inhalation monkey and guinea pig 14 ppm, 7 hr day⁻¹, 5 day wk⁻¹ for 106 days reduced body-weight gain and increased liver weight. No fatalities occurred (8).

Carcinogenicity and chronic effects

Reported to induce lung and stomach cancers in mice following repeated dermal application (9).

Irritancy

Dermal rabbit (24 hr) 500 mg caused moderate irritation and 100 mg instilled into rabbit eye caused mild irritation (exposure unspecified) (8).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA104 with metabolic activation positive (10).

Escherichia coli DNA polymerase-deficient strain positive (11).

Other effects

Other adverse effects (human)

Exposure to 16 ppm for 10 min caused near-fatal liver injury (12).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (13).

Other comments

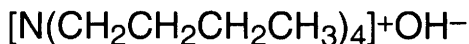
Physical properties, use, mammalian toxicity and safety precautions reviewed (14,15).

Autoignition temperature 335°C.

References

1. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
2. GEMS: *Graphical Exposure Modeling System. Fate of Atmospheric Pollutants* 1986, US EPA, Washington, DC, USA.
3. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
4. *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 251.
5. *AMA Arch. Ind. Hyg. Occup. Med.* 1950, **2**, 407.
6. *Vrachebroe Delo.* 1967, (3), 80.
7. Wolff, L. *Acta Biol. Med. Germanica* 1982, **41**, 945.
8. Hollingsworth, R. L. et al *Am. Ind. Hyg. Assoc. J.* 1963, **24**, 28.
9. van Duuren, B. L. et al *J. Natl. Cancer Inst.* 1979, **63**(6), 1433-1439.
10. Strobel, K. et al *Toxicol. Environ. Chem.* 1987, **15**, 101-128.
11. Rosenkranz, H. S. et al *Environ. Health Perspect.* 1977, **21**, 79-84.
12. Gosselin, R. E. et al *Clinical Toxicology of Commercial Products* 5th ed., 1984, **II**, 164, Williams & Wilkins, Baltimore, MD, USA.
13. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
14. *Chemical Safety Data Sheets* 1991, **4b**, 200-202, The Royal Society of Chemistry, London, UK.
15. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T41 tetrabutylammonium hydroxide



$\text{C}_{16}\text{H}_{37}\text{NO}$

Mol. Wt. 259.48

CAS Registry No. 2052-49-5

EINECS No. 218-147-6

RTECS No. BS 5425000

Uses Phase-transfer catalyst. Titrant in potentiometric titration.

Physical properties

M. Pt. 29.85°C Flash point 11°C Specific gravity 0.968

Solubility Water: >40%. Organic solvents: methanol

Environmental fate

Degradation studies

Degraded by *Nocardia* sp. in wastewaters. Not degraded by conventional methods (1).

Mammalian & avian toxicity

Acute data

LD_{50} subcutaneous mouse 19 mg kg^{-1} (2).

Other effects

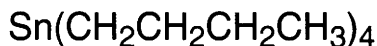
Other adverse effects (human)

Extremely destructive to tissue of the mucous membranes, upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema (3).

References

1. Oshimi, T. et al *Sumitomo Iukikai Envirotech. Inc.* Jpn. Kokai Tokkyo Koho JP 62, 104,573 [87, 104,573] (Cl. C12N1/20) 15 May 1987.
2. *J. Pharmacol. Exp. Therap.* 1926, **28**, 367.
3. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3237, Sigma-Aldrich, Milwaukee, WI, USA

T42 tetrabutyltin



$\text{C}_{16}\text{H}_{36}\text{Sn}$

Mol. Wt. 347.17

CAS Registry No. 1461-25-2

Synonyms tetrabutylstannane; tetra-*N*-butyltin

EINECS No. 215-960-8

RTECS No. WH 8605000

Uses Polymerisation catalyst. Organic synthesis. Lubricant and fuel additive. Stabilising and rust-inhibiting agent for silicones.

Physical properties

M. Pt. -97°C **B. Pt.** 127-145°C at 10 mmHg **Flash point** 107°C **Specific gravity** 1.055 at 25°C
Partition coefficient $\log P_{ow}$ 3.90 (1) **Volatility** v.p. 2.2×10^{-3} mmHg at 25°C
Solubility Organic solvents: diethyl ether, ethanol

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Sn) (total dust)
SE-LEVL 0.1 mg m⁻³ (as Sn) **SE-STEL** 0.2 mg m⁻³ (as Sn)
UK-LTEL 0.1 mg m⁻³ (as Sn) **UK-STEL** 0.2 mg m⁻³ (as Sn)
US-TWA 0.1 mg m⁻³ (as Sn) **US-STEL** 0.2 mg m⁻³ (as Sn)
UN No. 2788 (liquid)
UN No. 3146 (solid) **HAZCHEM Code** 2X (solid) **Conveyance classification** toxic substance

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) red killifish 52 mg l⁻¹ (2).

LC₅₀ (96 hr) fathead minnow 45 µg l⁻¹ flow-through bioassay (3).

Invertebrate toxicity

EC₅₀ (24 hr) *Daphnia magna* 0.61 mg l⁻¹ (1).

EC₅₀ (30 min) *Photobacterium phosphoreum* 0.001 ppm Microtox test (4).

Environmental fate

Abiotic removal

The Sn-C bond is susceptible to both nucleophilic and electrophilic attack. It may react with free radicals since the Sn-C bond is a good radical trap (5).

Mammalian & avian toxicity

Acute data

LD_{Lo} oral mouse 1400 mg kg⁻¹ (6).

LD_{Lo} dermal rabbit 2000 mg kg⁻¹ (7).

LD_{Lo} intraperitoneal mouse 170 mg kg⁻¹ (6).

LD_{Lo} intramuscular mouse 1400 mg kg⁻¹ (6).

LD₅₀ intravenous mouse 56 mg kg⁻¹ (8).

Metabolism and toxicokinetics

Following intravenous administration to ♂ rabbits, tetrabutyltin was slowly distributed to the liver. Partially converted into tributyltin (9).

Following oral administration to rats, high levels were detected in tissues of the gastro-intestinal tract, particularly the jejunum. Tributyltin was detected in the colon (10).

Irritancy

500 mg instilled into rabbit eye for 24 hr caused mild irritation (11).

Other effects

Other adverse effects (human)

Extremely destructive to tissues of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema (12).

Any other adverse effects

Oral mouse, single dose of 3000 mg kg⁻¹ caused liver damage which was manifested by elevated serum glutamic-pyruvic transaminase activity (13).

Oral administration to rabbits caused reversible anaemia. Iodine derivatives were more toxic (14).
Causes central nervous system damage, paralysis always starting at the posterior quarters in animals (15).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (16).
The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th Amendments) (17).

Other comments

Detected in natural waters and sediments (18).
Inhibited the activity of purified yeast glucose-6-phosphate dehydrogenase (19).
Physical properties, uses, occurrence, environmental impact and mammalian toxicology reviewed (3,20).

References

1. Vighi, M. et al *Chemosphere* 1987, **16**(5), 1043-1051.
2. Nagase, H. et al *Appl. Organometal. Chem.* 1991, **5**, 91-97.
3. *IPCS Environmental Health Criteria No. 15* 1980, WHO, Geneva, Switzerland.
4. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
5. Blunden, S. J. et al *Organometallic Compounds in the Environment* Craig, P. J. (Ed.), 1986, 136, John Wiley & Sons, New York, NY, USA.
6. *Annal. Pharmac. Francais* 1956, **14**, 88.
7. *Jpn. J. Ind. Health* 1973, **15**, 3.
8. *Report No. NX 02221* US Army Armaments Research and Development Command, Chemical Systems Laboratory, Aberdeen Proving Ground, MD, USA.
9. Arakawa, Y. et al *Toxicol. Appl. Pharmacol.* 1981, **60**(1), 1-7.
10. Boner, I. J. *Toxicology* 1989, **55**(3), 253-298.
11. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
12. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3240, Sigma-Aldrich, Milwaukee, WI, USA.
13. Calley, D. J. et al *J. Pharm. Sci.* 1967, **56**(2), 240-243.
14. Ando, M. et al *J. Tokyo Med. Coll.* 1961, **19**(5).
15. Lefaux, R. *Practical Toxicology of Plastics* 1968, 385, CRC Press, Cleveland, OH, USA.
16. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
17. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
18. Maguire, R. J. et al *Chemosphere* 1988, **15**, 253-274.
19. Kanetoshi, A. et al *Eisei Kagaku* 1981, **27**(3), 163-168.
20. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T43 1,1,3,3-tetrachloroacetone



$\text{C}_3\text{H}_2\text{Cl}_4\text{O}$

Mol. Wt. 195.86

CAS Registry No. 632-21-3

Synonyms 1,1,3,3-tetrachloro-2-propanone; tetrachloroacetone

EINECS No. 211-172-3

RTECS No. UC 3815100

Occurrence Isolated from *Asparogopsis toxiformis*.

Physical properties

B. Pt. 182°C **Specific gravity** 1.594 at 25°C with respect to water at 4°C
Solubility Organic solvents: acetone, dimethyl sulfoxide

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 180 mg kg⁻¹ (1).

LD₅₀ dermal rabbit 80 mg kg⁻¹ (1).

Teratogenicity and reproductive effects

Oral mouse, lowest toxic dose 500 mg kg⁻¹ day⁻¹ on days 6-15 of gestation (teratogenic effects to musculoskeletal system and craniofacial region) (1).

Oral rabbit, lowest toxic dose 130 mg kg⁻¹ day⁻¹ on days 6-18 of gestation (teratogenic effects to musculoskeletal system) (1).

Oral mouse, lowest toxic dose 150 mg kg⁻¹ day⁻¹ on days 6-15 of gestation (post-implantation mortality) (1).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537, TA1538 with metabolic activation positive (2).

Saccharomyces cerevisiae D7, XV 185-14C with and without metabolic activation positive (3).

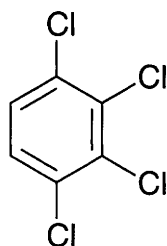
Other comments

Formed during bleaching on paper pulp (4,3).

References

1. *Fundam. Appl. Toxicol.* 1982, **2**, 220.
2. Nestmann, E. R. et al *Environ. Mutagen.* 1985, **7**, 163-170.
3. Nestmann, E. R. et al *Mutat. Res.* 1985, **155**, 53-60.
4. Priha, M. H. et al *Pulp Pap. Can.* 1986, **87**(12), 143-144, 147

T44 1,2,3,4-tetrachlorobenzene



C₆H₂Cl₄

Mol. Wt. 215.89

CAS Registry No. 634-66-2

Synonyms tetrachlorobenzene

EINECS No. 211-124-0

RTECS No. DB 9440000

Uses In dielectric fluids. Organic synthesis.

Physical properties

M. Pt. 46-47°C B. Pt. 254°C at 761 mmHg Flash point >112°C Partition coefficient $\log P_{ow}$ 3.5 (1)
Solubility Water: 3.5 mg l⁻¹ at 22°C. Organic solvents: acetone, acetic acid, carbon disulfide, diethyl ether, ethanol

Occupational exposure

SE-LEVL 0.5 mg m⁻³

SE-STEL 1.5 mg m⁻³

Ecotoxicity

Fish toxicity

LC₅₀ (14 day) guppy 0.8 mg l⁻¹ (2).

LC₅₀ (96 hr) fathead minnow 1.1 mg l⁻¹ flow-through bioassay (3).

LD₅₀ intraperitoneal rainbow trout 1100 mg kg⁻¹.

LC₅₀ rainbow trout 0.49 mg l⁻¹ (exposure unspecified) (4).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 4.0 ppm Microtox test (5).

LC₅₀ (24 hr) *Artemia* 4.3 mg l⁻¹ (6).

Bioaccumulation

Bioconcentration factor for rainbow trout 2,600-8,600 in 7-96 days (1).

Bioconcentration factor for bluegill sunfish 1820, 28 days at 16°C (7).

Environmental fate

Nitrification inhibition

IC₅₀ (25 day) *Nitrosomonas* sp. 20 mg l⁻¹ (8).

Anaerobic effects

IC₅₀ (50 day) methanogenic bacterial culture 20 mg l⁻¹ (8).

Degradation studies

Degraded by *Pseudomonas* sp. at 200 mg l⁻¹ at 30°C: 33% ring cleavage by parent strains after 120 hr; 74% ring cleavage by mutant strains after 120 hr (strains unspecified) (9).

Adsorption and retention

Soil sorption coefficient in clay loam, light clays and sandy loam soils, K_{oc} 3000-8100 (10).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, rabbit 1200, 1500 mg kg⁻¹, respectively (11,12).

Sub-acute and sub-chronic data

Oral rat 0, 0.5, 5.0, 50 or 500 ppm diet for 13 wk caused liver and kidney damage. Of the three isomers, 1,2,4,5-tetrachlorobenzene caused the most severe lesions (13).

Teratogenicity and reproductive effects

Oral rat, lowest toxic dose 1500 mg kg⁻¹ day⁻¹ on days 9-13 of gestation (foetotoxicity and extra-embryonic structure) (14).

Oral rat lowest toxic dose 2000 mg kg⁻¹ day⁻¹ on days 6-15 of gestation (reduced litter size) (15).

Gavage rat 0, 50, 100 or 200 mg kg⁻¹ day⁻¹ on days 5-15 gestation. No maternal toxicity or teratogenic effects were observed. The high dose caused a reduction in the number of foetuses (16).

Metabolism and toxicokinetics

Following oral administration to rats of ¹⁴C-labelled substance, radiolabel distributed to all tissue examined, with the highest concentrations found in the fat, liver, skin and adrenal gland. The decay rate in the tissues was 12 hr (17).

Following oral administration to monkeys of ^{14}C -labelled substance, 38% was excreted in the faeces within 48 hr. Unchanged compound accounted for 50% of faecal radioactivity. Metabolites identified were: 1,2,4,5-tetrachlorophenol (22%), *N*-acetyl-S-(2,3,4,5-tetrachlorophenyl)cysteine (18%), 2,3,4,5-tetrachlorophenyl sulfuric acid (3%), 2,3,4,5-tetrachlorophenyl methyl sulfoxide (0.6%) and 2,3,4,5-tetrachlorophenyl methyl sulfide (0.2%) (18).

Irritancy

Irritating to the skin, eyes, mucous membranes and upper respiratory tract (species unspecified) (19).

Genotoxicity

Salmonella typhimurium TA100 with and without metabolic activation negative (20).

In vitro Chinese hamster ovary cells, sister chromatid exchanges with metabolic activation positive, chromosomal aberrations with and without metabolic activation negative (21).

In vivo mouse bone marrow erythrocytes micronucleus test positive (22).

Legislation

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th amendments) (23).

Other comments

Detected in natural waters and sediments (24,25).

Detected in fat phase of fish, animal and human adipose tissue (26,27).

Excised soybean roots were exposed to an aqueous solution of 1,2,3,4-tetrachlorobenzene. Effective equilibration was reached within 2.5 hr and the elimination rate constant was $>4.1 \text{ hr}^{-1}$ (28).

Mammalian toxicology and health hazards reviewed (29,30).

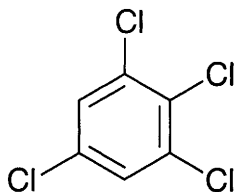
Technical grade contains 30% 1,2,4,5-isomer.

References

1. Oliver, B. G. et al *Environ. Sci. Technol.* 1985, **19**(9), 842-849.
2. Konemann, W. H. *Quantitative Structure-Activity Relationships for Kinetics and Toxicity of Aquatic Pollutants and their Mixtures in Fish* 1979, Univ. Utrecht, Netherlands.
3. Veith, G. D. et al *Can. J. Fish. Aquat. Sci.* 1983, **40**(6), 743-748.
4. Hodson, P. V. et al *Environ. Toxicol. Chem.* 1988, **7**, 443-454.
5. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
6. Abernethy, S. G. et al *Environ. Toxicol. Chem.* 1988, **7**, 469-481.
7. Garst, J. E. et al *J. Pharm. Sci.* 1984, **73**(11), 1616-1623.
8. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, **63**(3), 198-207.
9. Worne, H. E. *Tijdschrift van Let BECEWA* Liege, Belgium.
10. Kishi, H. et al *Chemosphere* 1990, **21**(7), 867-876.
11. Chu, I. et al *J. Toxicol. Environ. Health* 1983, **11**, 663-677.
12. Verschuere, K. *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, 1068, Van Nostrand Reinhold, New York, NY, USA.
13. Chu, I. et al *Drug Chem. Toxicol.* 1984, **7**(2), 113-127.
14. Kitchin, K. T. et al *Toxicology* 1993, **26**, 243-256.
15. Kacew, S. et al *Teratology* 1984, **29**, 21-27.
16. Kacew, S. et al *Teratology* 1984, **29**, 7-21.
17. Chu, I. et al *QSAR Environ. Toxicol. Proc. 2nd Int. Workshop* 1986, 55-60.
18. Schwartz, H. et al *J. Toxicol. Environ. Health* 1987, **22**(3), 341-350.
19. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3243, Sigma-Aldrich, Milwaukee, WI, USA.
20. Klopman, G. et al *Mol. Toxicol.* 1987, **17**, 61-81.
21. Loveday, K. S. et al *Environ. Mol. Mutagen.* 1990, **16**(4), 272-303.
22. Parrini, M. et al *Boll.-Soc. Ital. Biol. Sper.* 1990, **66**(7), 709-716.
23. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.

24. Biberhofer, J. et al *Sci. Ser. – Inland Waters/Land Dir. (Can.)* 1987, 159.
25. Kaiser, K. L. E. et al *Sci. Total Environ.* 1990, **97-98**, 495-506.
26. Ofstad, E. B. et al *Sci. Total Environ.* 1978, **10**, 219-230.
27. Williams, D. T. et al *J. Toxicol. Environ. Health* 1984, **13**(1), 19-29.
28. Kraaij, H. et al *Chemosphere* 1997, **34**(12), 2607-2620.
29. Peirano, W. B. *Report* 1985, EPA/600/8-84/015F Govt. Rep. Announce. Index (U.S.) 1985, **85**(6), 46 (*Chem. Abstr.* **102**, 216489p).
30. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T45 1,2,3,5-tetrachlorobenzene



$C_6H_2Cl_4$

Mol. Wt. 215.89

CAS Registry No. 634-90-2

Synonyms tetrachlorobenzene

EINECS No. 211-217-7

Uses Organic synthesis.

Physical properties

M. Pt. 50-52°C **B. Pt.** 246°C **Flash point** 155°C **Partition coefficient** $\log P_{ow}$ 4.94 (1)

Solubility Water: 2.4 mg l⁻¹ at 22°C. Organic solvents: benzene, carbon disulfide, diethyl ether, ethanol, petroleum ether

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) sheepshead minnow, fathead minnow, bluegill sunfish 3.7-6.4 mg l⁻¹ (2,3,4).

LC₅₀ (14 day) guppy 0.8 mg l⁻¹ (5).

LD₅₀ intraperitoneal rainbow trout 1650 mg kg⁻¹.

LC₅₀ rainbow trout 1.5 mg l⁻¹ (exposure unspecified) (6).

Invertebrate toxicity

EC₅₀ (48 hr) *Daphnia magna* 1.7-5.4 mg l⁻¹ (4,5).

EC₅₀ (30 min) *Photobacterium phosphoreum* 2.5 ppm Microtox test (7).

LC₅₀ (24 hr) *Artemia* 2.9 mg l⁻¹ (4).

Bioaccumulation

Bioconcentration factor in guppy 72,000 and in the bacterium *Liderocapsa treabii* 3000 (5).

Bioconcentration factor in bluegill sunfish 1800 (8).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1700-2300 mg kg⁻¹ (9).

Sub-acute and sub-chronic data

Oral rat 0, 0.5, 5.0, 50 or 500 ppm diet for 13 wk caused liver and kidney damage. Of the 3 isomers 1,2,4,5-tetrachlorobenzene caused the most severe lesions (10).

Teratogenicity and reproductive effects

Oral rat, lowest toxic dose 2000 mg kg⁻¹ day⁻¹ on days 6-15 of gestation (reduced litter size) (11).

Gavage rat 0, 50, 100 or 200 mg kg⁻¹ day⁻¹ on days 6-15 of gestation. No maternal toxicity or teratogenic effects were observed. The high dose caused a reduction in the number of foetuses (12).

Metabolism and toxicokinetics

Following oral administration to rats of ¹⁴C-labelled substance, radiolabel was distributed to all tissues examined, with the highest concentrations found in the fat, liver, skin and adrenal gland. 46-51% of 10 mg oral dose was excreted in the urine and faeces within 48 hr (13).

Following oral administration to monkeys of ¹⁴C-labelled substance 36% was excreted in the faeces within 48 hr. Unchanged substance accounted for >50% of faecal radioactivity. Faecal metabolites were: 2,3,4,5-tetrachlorophenol (2%); 2,3,4,6-tetrachlorophenol (14%); 2,3,5,6-tetrachlorophenol (9%); and 2,3,5,6-tetrachlorophenyl sulfinic acid (15%). No radioactivity was eliminated in the urine (14).

Irritancy

Irritating to the eyes, skin, mucous membranes and upper respiratory tract (species unspecified) (15).

Genotoxicity

In vitro Chinese hamster ovary cells sister chromatid exchanges and chromosomal aberrations with and without metabolic activation negative (16).

In vivo mouse bone marrow erythrocytes micronucleus test negative (17).

Legislation

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th Amendments) (18).

Other comments

Metabolite of hexachlorobenzene. Found in human adipose tissue (19).

Detected in natural waters and sediments (20,21).

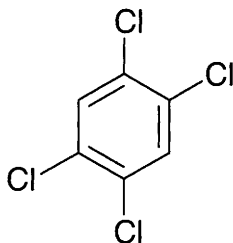
Mammalian toxicology and health hazards reviewed (22,23).

References

1. Vighi, M. et al *Chemosphere* 1987, **16**(5), 1043-1051.
2. *NIOSH Current Awareness Listing* 1985, Washington, DC, USA.
3. *Health Assessment Document: Chlorinated Benzenes* 1985, p6-6 EPA 600/8-84-015.
4. Abernethy, S. G. et al *Environ. Toxicol. Chem.* 1988, **7**, 469-481.
5. Konemann, W. H. *Quantitative Structure – Activity Relationships for Kinetics and Toxicity of Aquatic Pollutants and their Mixtures in Fish* 1979, Univ. Utrecht, Netherlands.
6. Abernethy, S. G. et al *Environ. Toxicol. Chem.* 1988, **7**, 443-454.
7. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
8. *Ambient Water Quality Criteria: Chlorinated Benzenes* 1980, 53, EPA 440/5-80-028.
9. Chu, I. et al *J. Toxicol. Environ. Health* 1983, **11**, 663-677.
10. Chu, I. et al *Drug Chem. Toxicol.* 1984, **7**(2), 113-127.
11. Kacew, S. et al *Teratology* 1984, **29**, 21-27.
12. Kacew, S. et al *Teratology* 1984, **29**, 7-21.
13. Chu, I. et al *QSAR Environ. Toxicol. Proc. 2nd Int. Workshop* 1986, 55-60.
14. Schwartz, H. et al *J. Toxicol. Environ. Health* 1987, **22**(3), 341-350.
15. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3243, Sigma-Aldrich, Milwaukee, WI, USA.
16. Loveday, K. S. et al *Environ. Mol. Mutagen.* 1990, **16**(4), 272-303.
17. Parrini, M. et al *Boll. – Soc. Ital. Biol. Sper.* 1990, **66**(7), 709-716.
18. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; *6th Amendment EEC Directive* 79/831/EEC; *7th Amendment EEC Directive* 91/32/EEC 1991, HMSO, London, UK.

19. Williams, D. T. et al *J. Toxicol. Environ. Health* 1984, **13**(1), 19-29.
20. Biberhofer, J. et al *Sci., Ser. – Inland Waters/Land Dir. (Can.)* 1987, 159.
21. Kaiser, K. L. E. et al *Sci. Total Environ.* 1990, **97-98**, 495-506.
22. Peirano, W. B. *Report* 1985, **85**(6), 46 (*Chem. Abstr.* **102**, 216489p).
23. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T46 1,2,4,5-tetrachlorobenzene



$C_6H_2Cl_4$

Mol. Wt. 215.89

CAS Registry No. 95-94-3

Synonyms TCB; tetrachlorobenzene

EINECS No. 202-466-2

RTECS No. DB 9450000

Uses Fungicide. Synthesis of herbicides. Electrical insulator. Impregnator for moisture resistance.

Physical properties

M. Pt. 138°C B. Pt. 245°C Flash point >110°C Specific gravity 1.858 at 21°C with respect to water at 4°C

Partition coefficient $\log P_{ow}$ 4.70 Volatility v.p. 40 mmHg at 146°C; v.den. 7.4

Solubility Water: 0.3 mg l⁻¹ at 22°C. Organic solvents: acetonitrile, benzene, chloroform, diethyl ether, ethanol

Ecotoxicity

Fish toxicity

LC₅₀ (14 day) guppy 0.3 mg l⁻¹ (1).

LC₅₀ (96 hr) fathead minnow, bluegill sunfish 1.55 mg l⁻¹ (2,3).

LC₅₀ (96 hr) American flagfish 1.8-2.5 mg l⁻¹ – flow-through bioassay (4).

Invertebrate toxicity

EC₅₀ (40 min) *Photobacterium phosphoreum* 4.5 ppm Microtox test (5).

Bioaccumulation

Bioconcentration factor for fish 4500 (species unspecified). This compares with a calculated value of 225 (6).

Environmental fate

Nitrification inhibition

IC₅₀ (25 day) *Nitrosomonas* 9.8 mg l⁻¹ (7).

Degradation studies

Degraded by *Pseudomonas* sp. at 200 mg l⁻¹ at 30°C: 30% ring cleavage by parent strains in 120 hr, 80% ring cleavage by mutant strains in 120 hr (8).

Utilised as sole carbon source by *Pseudomonas* sp.

Catabolism involves dioxygenation to form 1,3,4,6-tetrachloro-1,2-dihydroxycyclohexa-3,5-dione, followed by elimination of hydrogen chloride and ortho-cleavage (9).

Abiotic removal

Exposure of 20 g to sunlight yielded 26 ppm polychlorinated biphenyl products (10).

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated $t_{1/2}$ 190 days (11).

Volatilisation $t_{1/2}$ 4.8 hr from model river water, 59.3 days from model pond water (12,13).

Adsorption and retention

K_{oc} 5200-8500 in soils containing 0.06-0.73% organic content (14).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat, rabbit 1000, 1500, 3100 mg kg⁻¹, respectively (15,16).

Sub-acute and sub-chronic data

Oral rat 500 ppm diet for 21 days caused no deaths. Increased liver weight, serum cholesterol and hepatic enzyme activity were reported. Moderate to severe histological changes to the liver, thyroid, kidneys and lungs were observed. The 1,2,4,5-isomer was reported to be accumulated much more rapidly in the organs than the 1,2,3,4- and 1,2,3,5-isomers (16).

Oral rat 0, 0.5, 5.0, 50 or 500 ppm diet for 13 wk caused liver and kidney damage. Of the 3 isomers, 1,2,4,5-tetrachlorobenzene caused the most severe lesions (17).

Teratogenicity and reproductive effects

Gavage rat 0, 50, 100 or 200 mg kg⁻¹ day⁻¹ on days 6-13 of gestation. The high dose caused the death of 9/10 dams. The number of foetuses was reduced but no teratogenic effects were observed (18).

Metabolism and toxicokinetics

In rats faecal and urinary metabolites included 2,3,5,6-tetrachlorophenol, tetrachloroquinol and trichlorophenol. 8% of 10 mg kg⁻¹ oral dose was excreted in the urine and faeces within 48 hr (16,19).

Following oral administration to rats of ¹⁴C-labelled substance, radiolabel was distributed to all tissues examined, with the highest concentrations found in the fat, liver, skin and adrenal gland. The decay rate in the tissues was 105 hr (19).

Following oral administration of ¹⁴C-labelled substance to monkeys, 18% of the radiolabel was excreted in the faeces within 48 hr. The material was excreted in the faeces unchanged. No radioactivity was detected in the urine (20).

Irritancy

Irritating to the eyes, skin, mucous membranes and upper respiratory tract (species unspecified) (21).

Genotoxicity

Salmonella typhimurium TA100 with metabolic activation negative (22).

Drosophila melanogaster sex-linked recessive lethal assay positive (23).

In vitro Chinese hamster ovary cells, sister chromatid exchanges and chromosomal aberrations with and without metabolic activation negative (24).

In vivo mouse bone marrow erythrocytes micronucleus test positive (25).

Legislation

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th Amendments) (26). Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (27).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (28).

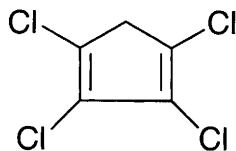
Other comments

Metabolite of hexachlorobenzene. Found in human adipose tissue (29).
Residues have been isolated from natural waters and sediments (30,31).
Mammalian toxicology and health hazards reviewed (32,33).

References

1. Konemann, W. H. *Quantitative Structure – Activity Relationships for Kinetics and Toxicity of Aquatic Pollutants and their Mixtures in Fish* 1979, Univ. Utrecht, Netherlands.
2. *Health Assessment Document: Chlorinated Benzenes* 1985, EPA 600/8-84-015.
3. Hall, L. H. et al *Environ. Toxicol. Chem.* 1989, **8**, 783-788.
4. Smith, A. D. et al *Arch. Environ. Contam. Toxicol.* 1991, **20**, 94-102.
5. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
6. Sabladjic, A. et al *Chem. – Biol. Interact.* 1982, **42**, 301-310.
7. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, **63**(3), 198-207.
8. Worne, H. E. *Tijdschrift van Let CECEWA* Liege, Belgium.
9. Sander, P. et al *Appl. Environ. Microbiol.* 1991, **57**(5), 1430-1440.
10. Uyeta, M. et al *Nature (London)* 1976, **264**, 583.
11. Atkinson, R. et al *Environ. Sci. Technol.* 1987, **21**, 64-72.
12. *EXAMS II Computer Simulation* 1987, US EPA, Athens, GA, USA.
13. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
14. Schuartenbach, R. P. et al *Environ. Sci. Technol.* 1980, **4**, 31.
15. *Hyg. Sanit.* 1965, **30**, 8.
16. Chu, I. et al *J. Toxicol. Environ. Health* 1983, **11**, 663-677.
17. Chu, I. et al *Drug. Chem. Toxicol.* 1984, **7**(2), 113-127.
18. Kacew, S. et al *Teratology* 1984, **29**, 7-21.
19. Chu, I. et al *QSAR Environ. Toxicol. Proc. 2nd Int. Workshop* 1986, 55-60.
20. Schwartz, H. et al *J. Toxicol. Environ. Health* 1987, **22**(3), 341-350.
21. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3243, Sigma-Aldrich, Milwaukee, WI, USA.
22. Klopman, G. et al *Mol. Toxicol.* 1987, **17**, 61-81.
23. Paradi, E. et al *Acta Biol. Acad. Sci. Hung.* 1981, **32**(2), 119-122.
24. Loveday, K. S. et al *Environ. Mol. Mutagen.* 1990, **16**(4), 272-303.
25. Parrini, M. et al *Boll. - Soc. Ital. Biol. Sper.* 1990, **66**(7), 709-716.
26. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
27. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
28. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
29. Williams, D. T. et al *J. Toxicol. Environ. Health* 1984, **13**(1), 19-29.
30. Miller, M. M. et al *J. Chem. Eng. Data* 1984, **29**(2), 184-190.
31. Oliver, B. G. et al *Sci. Total Environ.* 1984, **16**, 532.
32. Peirano, W. B. *Report* 1985, EPA/600/8-84/015F, from *Govt. Rep. Announce. Index (U.S.)* 1985, **85**(6), 46 (*Chem. Abstr.* **102**, 216489p).
33. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T47 1,2,3,4-tetrachloro-1,3-cyclopentadiene



$C_5H_2Cl_4$

Mol. Wt. 203.88

CAS Registry No. 695-77-2

Synonyms tetrachlorocyclopentadiene

RTECS No. GY 1577000

Uses Organic synthesis.

Physical properties

M. Pt. 58°C B. Pt. 62-63°C

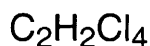
Genotoxicity

Escherichia coli K12 with metabolic activation positive (1).

References

1. Goggelman, W. et al *Biochem. Pharmacol.* 1978, 27, 2927-2929

T48 tetrachloroethane



$C_2H_2Cl_4$

Mol. Wt. 167.85

CAS Registry No. 25322-20-7

EINECS No. 246-842-4

RTECS No. KI 8400000

Uses Solvent.

Physical properties

B. Pt. 146°C Partition coefficient $\log P_{ow}$ 2.39 (1)

Solubility Organic solvents: acetone, benzene, chloroform, diethyl ether, ethanol

Occupational exposure

UN No. 1702 HAZCHEM Code 2XE Conveyance classification toxic substance

Ecotoxicity

Invertebrate toxicity

EC₅₀ (5 min) *Photobacterium phosphoreum* 8.6 ppm Microtox test (2).

Environmental fate

Degradation studies

Tetrachloroethane is reductively dechlorinated to *cis*-1,2-dichloroethene by cell extracts of *Desulfotobacterium* sp. strain PCE-S. The enzyme tetrachloroethane dehalogenase catalyses this reaction and requires the involvement of a corrinoid (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 320 mg kg⁻¹ (4).

LC₅₀ (4 hr) inhalation rat 1000 ppm (4).

LD₅₀ dermal rabbit 6300 mg kg⁻¹ (4).

LD_{Lo} intraperitoneal guinea pig 500 mg kg⁻¹ (4).

Teratogenicity and reproductive effects

Application via mouse skin, lowest toxic dose 3200 mg kg⁻¹ day⁻¹ (post-implantation mortality) (exposure period not specified) (5).

Genotoxicity

In vitro Chinese hamster V79 cells, disturbances in spindle formations (C-mitosis) and induction of aneuploidy positive (1).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (6).

References

1. Onfelt, A. *Mutat. Res.* 1987, **182**, 135-154.
2. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
3. Miller, E. et al *Arch. Microbiol.* 1997, **168**(6), 513-519.
4. *Am. Int. Hyg. Assoc. J.* 1969, **30**, 470.
5. *Biologische Rundschau* 1976, **14**, 220.
6. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T49 1,1,1,2-tetrachloroethane



C₂H₂Cl₄

Mol. Wt. 167.85

CAS Registry No. 630-20-6

Synonyms NCI-C52459; 1,2,2,2-tetrachloroethane; tetrachloroethane

EINECS No. 211-135-1

RTECS No. KI 8450000

Uses Solvent.

Physical properties

M. Pt. -70.2°C B. Pt. 138°C Specific gravity 1.598 at 20°C with respect to water at 4°C

Partition coefficient log P_{ow} 3.1933 (1) Volatility v.p. 12.03 mmHg at 25°C

Solubility Water: 1100 mg l⁻¹ at 25°C. Organic solvents: acetone, benzene, chloroform, diethyl ether, ethanol

Occupational exposure

UN No. 1702 HAZCHEM Code 2XE Conveyance classification toxic substance

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bluegill sunfish 20 mg l⁻¹ (2).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 2.8 ppm Microtox test (3).

Bioaccumulation

Estimated bioconcentration of 12 indicates that environmental accumulation is unlikely (4).

Environmental fate

Nitrification inhibition

IC₅₀ (25 day) *Nitrosomonas* sp. 8.7 mg l⁻¹ (5).

Carbonaceous inhibition

IC₅₀ (5 day) aerobic heterotrophs isolated from activated sludge 230 mg l⁻¹ (5).

Anaerobic effects

IC₅₀ (50 day) methanogenic bacterial culture 1.7 mg l⁻¹ (5).

Abiotic removal

Estimated hydrolysis t_{1/2} >50 yr (6).

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated t_{1/2} 550 days (7).

Volatilisation from model river water, estimated t_{1/2} 4.2 hr (4).

Adsorption and retention

Calculated K_{oc} of 93 indicates moderate adsorption to soil and sediments (4).

Experimentally determined K_{oc} 399 (8).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 670, 1500 mg kg⁻¹, respectively (9).

LC₅₀ (4 hr) inhalation rat, rabbit 2100, 2800 ppm, respectively (9).

LD₅₀ dermal rabbit 20,000 mg kg⁻¹ (9).

Sub-acute and sub-chronic data

Oral rat 300 mg kg⁻¹ day⁻¹, 5 days wk⁻¹ for 2 wk caused hepatic steatosis. 400 mg dosages caused 10% mortality in ♂ and 20% mortality in ♀ rats (10).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (11).

Oral rat, mouse (2 yr) 0, 250 or 500 mg kg⁻¹ day⁻¹ 5 days wk⁻¹ for mice, 0, 125, or 250 mg kg⁻¹ day⁻¹ 5 days wk⁻¹ for rats. Clinical signs of central nervous system toxicity were seen in high-dose mice and in both treated groups of rats. There was a statistically significant dose-related incidence of hepatocellular adenomas in ♂ and ♀ mice, hepatocellular carcinomas in ♀ mice, and fibroadenomas of the mammary gland in ♀ rats (12).

Metabolism and toxicokinetics

Following subcutaneous administration to mice, 21-62% was eliminated unchanged in exhaled air. The major urinary metabolite (17-49%) was trichloroethanol and its glucuronide conjugate. Trichloroacetic acid (1-7%) was also excreted in the urine. These urinary metabolites were also identified in rats and guinea pigs (13-15).

In the presence of oxygen, NADPH and rat liver microsomes *in vitro*, 1,1,1,2-tetrachloroethane undergoes little dechlorination. In contrast, NADPH-dependent reductive metabolism by microsomal fractions yields 1,1-dichloroethylene as the major metabolite and 1,1,2-trichloroethane as a minor metabolite (16-19).

Irritancy

Dermal rabbit (24 hr) 500 mg caused irritation and 100 mg instilled into rabbit eye caused severe irritation (exposure unspecified) (9).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538 with and without metabolic activation negative (20,21).

In vitro mouse lymphoma L5178Y cells tk⁺/tk⁻ forward mutation assay positive with and without metabolic activation (22).

In vitro Chinese hamster ovary cells sister chromatid exchanges positive, chromosomal aberrations negative with and without metabolic activation (23,24).

In vitro BALB/C-3T3 clone 1-13 cell transformations negative (25).

Aspergillus nidulans gene mutations, mitotic crossing over, chromosomal malsegregation and aneuploidy positive with and without metabolic activation (26).

Legislation

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th Amendments) (27).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (28).

US EPA recommended maximum concentration in fresh water 9.32 mg l⁻¹ (29).

Other comments

Detected in natural water, sediments, air samples and in human tissues (30,31).

Environmental fate reviewed (30).

Physical properties, uses, occurrence, analysis, carcinogenicity, mammalian toxicology, metabolism and mutagenicity reviewed (31).

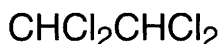
Reviews on human health effects, experimental toxicology, physico-chemical properties listed (32).

References

1. McCoy, G. D. et al *Carcinogenesis* 1990, **11**(7), 1111-1117.
2. Buccafusco, R. J. et al *Bull. Environ. Contam. Toxicol.* 1981, **26**(4), 446-452.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
5. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, **63**(3), 198-207.
6. Mabey, W. R. et al *Symp. Am. Chem. Soc. Div. Environ. Chem.* 186th Natl. Mtg., Washington, DC, USA.
7. Atkinson, R. *Int. J. Chem. Kinet.* 1987, **19**, 799-828.
8. Rao, P. S. C. et al *J. Environ. Qual.* 1985, **14**, 376-383.
9. *Arch. Malad. Prof. Med. Terail Soc. Sec.* 1974, **35**, 593.
10. Truhaut, R. et al *J. Eur. Toxicol.* 1974, **7**, 81-84.
11. *IARC Monograph* 1987, **Suppl. 7**, 72.
12. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-237, NIEHS, Research Triangle Park, NC, USA.
13. Yllner, S. *Acta Pharmacol. Toxicol.* 1971, **29**, 471-480.
14. Ikeda, M. et al *Br. J. Ind. Med.* 1972, **29**, 99-104.
15. Truhaut, R. et al *J. Eur. Toxicol.* 1973, **4-5**, 211-217.
16. Van Dyke, R. A. et al *Biochem. Pharmacol.* 1971, **20**, 463-470.
17. Thompson, J. A. et al *Chem.-Biol. Interact.* 1984, **51**, 321-333.
18. Thompson, J. A. et al *Anal. Biochem.* 1985, **145**, 376-384.
19. Town, C. et al *Drug Metab. Dispos.* 1984, **12**, 4-8.
20. Haworth, S. et al *Environ. Mol. Mutagen.* 1983, **5**(Suppl. 1), 3-142.
21. Limmon, V. F. et al in *Progress in Genetic Toxicology* Scott, D. et al (Eds.) 1977, 244-258, Elsevier, Amsterdam, Netherlands.
22. McGregor, D. B. et al *Environ. Mol. Mutagen.* 1988, **12**, 437-442.
23. Zeiger, E. et al *Environ. Mol. Mutagen.* 1990, **16**(Suppl. 18), 1-14.

24. Galloway, S. M. et al *Environ. Mol. Mutagen.* 1987, **10**(Suppl. 10), 1-175.
25. Tu, A. S. et al *Cancer Lett.* 1985, **28**, 85-92.
26. Crebelli, R. et al *Proc. ICMR Lemini*. 1988, **8**, 437-442.
27. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
28. S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations 1991, HMSO, London, UK.
29. US EPA Ambient Water Quality Criteria for Chlorinated Ethanes 1980, PB81-117400, Washington, DC, USA.
30. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1991, **2**, 405-409, Lewis Publishers, Chelsea, MI, USA.
31. IARC Monograph 1986, **41**, 87-97.
32. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T50 1,1,2,2-tetrachloroethane



$\text{C}_2\text{H}_2\text{Cl}_4$

Mol. Wt. 167.85

CAS Registry No. 79-34-5

Synonyms Acetosan; acetylene tetrachloride; Bonaform; Cellon; 1,1-dichloro-2,2-dichloroethane; sym-tetrachloroethane; Westron; tetrachloroethane; NCI-C03554

EINECS No. 201-197-8

RTECS No. KI 8575000

Uses Solvent. Organic intermediate. Mothproofing agent for textiles. Fumigant.

Physical properties

M. Pt. -43°C **B. Pt.** 147°C **Specific gravity** 1.58658 at 25°C with respect to water at 4°C

Partition coefficient log P_{ow} 2.39 **Volatility** v.p. 6.1 mmHg at 25°C; v.den. 5.79

Solubility Water: 3000 mg l⁻¹ at 25°C. Organic solvents: benzene, chloroform, carbon disulfide, carbon tetrachloride, dimethylformamide, ethanol, oils

Occupational exposure

DE-MAK 1 ppm (7.0 mg m⁻³)

FR-VME 1 ppm (7 mg m⁻³)

FR-VLE 5 ppm (35 mg m⁻³)

JP-OEL 1 ppm (6.9 mg m⁻³)

US-TWA 1 ppm

UN No. 1702 **HAZCHEM Code** 2XE **Conveyance classification** toxic substance

Supply classification very toxic, dangerous for the environment

Risk phrases Very toxic by inhalation and in contact with skin – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R26/27, R51/53)

Safety phrases Restricted to professional users – Keep locked up and out of the reach of children (if sold to general public) – In case of insufficient ventilation, wear suitable respiratory equipment – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S38, S45, S61)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow, American flagfish 16-20 mg l⁻¹ – flow-through bioassay (1,2).

LC₅₀ (7 day) guppy 37 ppm (3).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 7.9 ppm Microtox test (4).

Bioaccumulation

Bioconcentration factor in bluegill sunfish 7.9 (5).

Environmental fate**Nitrification inhibition**

IC₅₀ (25 day) *Nitrosomonas* sp. 1.4 mg l⁻¹ (1).

Carbonaceous inhibition

IC₅₀ (5 day) aerobic heterotrophs isolated from activated sludge 130 mg l⁻¹ (1).

Anaerobic effects

IC₅₀ (50 day) methanogenic bacterial culture 4.1 mg l⁻¹ (1).

Degradation studies

41% degradation in 24 days in modified shake flask biodegradability test using unacclimated inoculum. 19% degradation in river bioassay test (6).

Abiotic removal

Degraded following pseudo 1st-order kinetics in anoxic sediment suspensions (7).

Volatilisation t_{1/2} in model river water 6.3 hr, and in model pond water 3.5 days (8,9).

Adsorption and retention

K_{oc} 79 in a silt loam soil (10).

Mammalian & avian toxicity**Acute data**

LD₅₀ oral rat 250-800 mg kg⁻¹ (11,12).

LC₅₀ (2 hr) inhalation mouse 4500 mg m⁻³ (12).

LD₅₀ subcutaneous mouse 1100 mg kg⁻¹ (13).

LD₅₀ intraperitoneal mouse 820 mg kg⁻¹ (14).

Sub-acute and sub-chronic data

Inhalation mouse (2 hr) 40 mg m⁻³ caused marked changes in lipid and ATP levels in the liver (15).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (16).

Gavage mouse (90 wk) 10 or 200 mg kg⁻¹ 5 day wk⁻¹ for 18 wk when doses were increased to 150 and 300 mg kg⁻¹, respectively. 3 wk later the doses were further increased to 200 and 400 mg kg⁻¹, respectively, which continued for 5 wk. A significant dose-related increase in the incidence of hepatocellular carcinomas was observed. In mice similarly treated with 50-130 mg kg⁻¹ there was no significant difference in the incidence of any tumours compared with controls (17).

Intraperitoneal mouse (24 wk) 0, 80, 200 or 400 mg kg⁻¹, 3 × wk⁻¹ for 6 wk. Survival rates were 10/20, 15/20 and 5/20, respectively, after 24 wk. The average numbers of lung tumours were 0.3, 0.5 and 1.0 mouse⁻¹ which were not significantly different from the 0.27 mouse⁻¹ in vehicle controls (18).

Teratogenicity and reproductive effects

Treatment of mice with 300-400 mg kg⁻¹ day⁻¹ for various periods during gestation produced dose-related embryotoxic effects and a low incidence of malformations (exencephaly, cleft palate, anophthalmia, fused ribs and vertebrae) (route of administration and total exposure unspecified) (19).

Metabolism and toxicokinetics

May be absorbed by inhalation, ingestion or through the skin of mammals (20).

Rapidly metabolised following intraperitoneal administration to mice. 50% of the ¹⁴C-labelled dose was expired as carbon dioxide, <4% expired, as unchanged 1,1,2,2-tetrachloroethane, with minute amounts of tri- and tetrachloroethylene. ~30% was excreted in the urine as di- and trichloroacetic acid, trichloroethanol, oxalic acid

and small amounts of glyoxalic acid and urea. ~50% of the radioactivity in the urine was unaccounted for. 16% of the administered dose was retained in the body (21).

Irritancy

Vapour or mist is irritating to the eyes, mucous membranes and upper respiratory tract (species unspecified) (22).

Sensitisation

Repeated exposure can cause dermatitis (species unspecified) (22,23).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538 with and without metabolic activation negative (24,25).

Saccharomyces cerevisiae with and without metabolic activation gene conversion homozygosis and reverse mutation positive (26).

Drosophila melanogaster sex-linked recessive lethal assay negative (27).

In vitro Chinese hamster ovary cells, sister chromatid exchanges positive, chromosomal aberrations negative (28).

In vitro BALB/C 3T3 cells (clone A-31) cell transformation with and without metabolic activation positive (29).

In vivo rat liver foci induction positive (30)

In vivo rat and mouse hepatocytes unscheduled DNA synthesis equivocal results (31).

Aspergillus nidulans gene mutations, mitotic crossing over, chromosomal malsegregation and aneuploidy negative (32).

Other effects

Other adverse effects (human)

Powerful narcotic and liver poison (33).

Among 3859 persons exposed to the solvent, slight excesses were reported for leukaemia and cancers of the genital organs, but these excesses were not significant (34).

Numerous deaths have been reported following ingestion, inhalation and cutaneous absorption, affecting primarily the central nervous system and the liver causing polyneuritis and paralysis (35).

Of 380 exposed workers 35% exhibited tremors and other nervous symptoms (36).

Accidental and occupational exposure produced liver damage, ranging from severe fatty degeneration to necrosis and acute atrophy, which was frequently fatal, and gastro-intestinal disorders. Toxic effects were also observed in the haematopoietic system (36).

Any other adverse effects

Oral rat single dose of 440 mg kg⁻¹ reduced hepatic benzo[*a*]pyrene-hydroxylase and *p*-nitroanisole-*o*-demethylase activities by 50% after 24 hr. Uridine 5'-diphosphate-glucuronyl transferase activity was reduced to a lesser extent (37).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (38).

Included in Schedule 4 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (39).

Other comments

Has been detected in urban air, drinking water and in some foods (35,40).

Physical properties, uses, occurrence, analysis, carcinogenicity, mammalian toxicology, metabolism and mutagenicity reviewed (35,24,41).

Environmental fate reviewed (40).

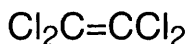
Has the highest solvent power of the chlorinated hydrocarbons (34).

Pharmacokinetics and implication in induction of mouse liver tumours reviewed (42).

References

1. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, **63**(3), 198-207.
2. Smith, A. D. et al *Arch. Environ. Contam. Toxicol.* 1991, **20**, 94-102.
3. Konemann, W. H. *Quantitative Structure – Activity Relationships for Kinetics and Toxicity of Aquatic Pollutants and their Mixtures in Fish* 1979, Univ. Utrecht, Netherlands.
4. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
5. Veith, G. D. et al *Science* 1979, **206**, 831-832.
6. Mudder, T. I. *Am. Chem. Soc. Div. Environ. Chem. Conf., Kansas City* 1982, 52-53.
7. Jafvert, C. T. et al *Environ. Toxicol. Chem.* 1987, **6**(11), 827-837.
8. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
9. *EXAMS II Computer Simulation* 1987, US EPA, Athens, GA, USA.
10. Chiou, C. T. et al *Science* 1979, **206**, 831-832.
11. Gahlke, R. et al *Z. Ges. Hyg.* 1977, **23**, 278-282.
12. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
13. *J. Pharmacol. Exp. Therap.* 1958, **123**, 224.
14. Takeuchi, Y. *Jpn. J. Ind. Health* 1966, **8**, 371-374.
15. Tomakuri, K. *Acta Med. Okayama* 1969, **23**, 273-282.
16. *IARC Monograph* 1987, **Suppl. 7**, 354-355.
17. National Cancer Institute *Bioassay of 1,1,2,3-Tetrachloroethene for Possible Carcinogenicity* 1978, Washington, DC, USA.
18. Theiss, J. C. et al *Cancer Res.* 1977, **37**, 2717-2720.
19. Schmidt, R. *Biol. Rundschau* 1976, **14**, 220-223.
20. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
21. Yllner, S. *Acta Pharmacol. Toxicol.* 1971, **29**, 499-512.
22. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3247, Sigma-Aldrich, Milwaukee, WI, USA.
23. *Chemical Safety Data Sheets* 1991, **4b**, 203-206, The Royal Society of Chemistry, London, UK.
24. Haworth, S. et al *Environ. Mol. Mutagen.* 1983, **5**(Suppl. 1), 3-142.
25. Nestmann, E. R. et al *Mutat. Res.* 1980, **79**, 203-212.
26. Woodruff, R. C. et al *Environ. Mol. Mutagen.* 1985, **7**, 677-702.
27. Callen, D. F. et al *Mutat. Res.* 1980, **77**, 55-63.
28. Galloway, S. M. et al *Environ. Mol. Mutagen.* 1987, **10**(Suppl. 10), 1-175.
29. Calci, A. et al *Jpn. J. Cancer Res.* 1990, **81**(8), 786-792.
30. Milmen, H. A. et al *Ann. N. Y. Acad. Sci.* 1988, **534**, 521-530.
31. Minsalis, J. C. et al *Environ. Mol. Mutagen.* 1989, **14**(3), 155-164.
32. Crebelli, R. et al *Proc. ICMR Lemin.* 1988, **8**, 437-442.
33. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
34. Norman, J. E. et al *J. Occup. Med.* 1981, **23**, 818-822.
35. *IARC Monograph* 1979, **20**, 478-489.
36. Labo-Mendonza, R. *Port. J. Ind. Med.* 1963, **20**, 50-56.
37. Vainio, H. et al *Xenobiotica* 1976, **6**, 599-604.
38. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
39. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
40. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1991, **2**, 410-417, Lewis Publishers, Chelsea, MI, USA.
41. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
42. Bolt, H. M. *Arch. Toxicol. Suppl.* 1987, **10**, 190-203

T51 tetrachloroethylene



C_2Cl_4

Mol. Wt. 165.83

CAS Registry No. 127-18-4

Synonyms Antisol 1; carbon bichloride; ethylene tetrachloride; Nema; perchloroethylene; Perclene; Percosalve; Tetracap; tetrachloroethene; tetrachloroethyleneum; Tetralex; Tetropil

EINECS No. 204-825-9

RTECS No. KX 3850000

Uses Solvent. Has been used as an anthelmintic and in the treatment of fasciolopsiasis.

Physical properties

M. Pt. -22°C **B. Pt.** 121°C **Specific gravity** 1.6230 at 20°C with respect to water at 4°C

Partition coefficient $\log P_{\text{ow}}$ 1.6647 (1) **Volatility** v.p. 20 mmHg at 26.3°C ; v.den. 5.83

Solubility Water: 150 mg l^{-1} at 25°C . Organic solvents: benzene, chloroform, diethyl ether, ethanol

Occupational exposure

FR-VME 50 ppm (335 mg m^{-3})

JP-OEL 50 ppm (340 mg m^{-3})

SE-LEVL 10 ppm (70 mg m^{-3})

SE-STEL 25 ppm (170 mg m^{-3})

UK-LTEL 50 ppm (345 mg m^{-3})

UK-STEL 100 ppm (689 mg m^{-3})

US-TWA 25 ppm (170 mg m^{-3})

US-STEL 100 ppm (685 mg m^{-3})

UN No. 1897 **HAZCHEM Code** 2 $\frac{+}{-}$ **Conveyance classification** toxic substance

Supply classification harmful

Supply classification dangerous for the environment

Risk phrases Possible risk of irreversible effects – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R40, R51/53)

Safety phrases Keep out of reach of children (if sold to general public) – Do not breathe vapour – Wear suitable protective clothing and gloves – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S23, S36/37, S61)

Ecotoxicity

Fish toxicity

LC_{50} (96 hr) fathead minnow, American flagfish 6.8, 17 mg l^{-1} , respectively – flow-through bioassay (2,3).

LC_{50} (17 day) guppy 18 mg l^{-1} (4).

Invertebrate toxicity

EC_{50} (30 min) *Photobacterium phosphoreum* 120 ppm Microtox test (5).

EC_{50} (24 hr) *Daphnia magna* 0.5 mg l^{-1} (6).

Bioaccumulation

Bioconcentration factor for fathead minnow, rainbow trout and bluegill sunfish 39-49 (7,8).

Environmental fate

Nitrification inhibition

IC_{50} (25 day) *Nitrosomonas* sp. 110 mg l^{-1} (2).

Carbonaceous inhibition

IC_{50} (5 day) aerobic heterotrophs isolated from activated sludge 1900 mg l^{-1} (2).

Anaerobic effects

IC_{50} (50 day) methanogenic bacterial culture 22 mg l^{-1} (2).

Degradation studies

24-76% degradation in anaerobic degradation studies, yielding trichloroethylene (9-11).

No biodegradation occurred in 21 days with acclimated or unacclimated inocula or in a river dia-assay test (12).

Abiotic removal

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated $t_{1/2}$ 2 months (13).

Volatilisation $t_{1/2}$ 3 hr-7 days in river water and 3.6-14 days in lake and pond water (14).

Adsorption and retention

Measured K_{oc} 210 (15,16).

Mammalian & avian toxicity**Acute data**

LD₅₀ oral rat, mouse 2600, 8100 mg kg⁻¹, respectively (17,18).

LC₅₀ (8 hr) inhalation rat 34,000 mg m⁻³ (17).

LD₅₀ intraperitoneal mouse, dog 2100, 47,000 mg kg⁻¹, respectively (19,20).

LD_{Lo} intravenous dog 85 mg kg⁻¹ (21).

Sub-acute and sub-chronic data

Inhalation rat 4000 mg m⁻³ for 6 hr day⁻¹, 5 days wk⁻¹ for 12 months resulted in reversible liver toxicity (22).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2B (23).

Oral rat and mouse, maximum tolerated dose 720 and 1070 mg kg⁻¹ day⁻¹, respectively, for 78 wk (24).

Oral mouse (90 wk) 300-311 mg kg⁻¹ day⁻¹ for 78 wk caused a significant increase in the incidence of hepatocellular carcinomas compared with controls (24).

Oral rat (110 wk) 500-1400 mg kg⁻¹ day⁻¹ for 78 wk did not cause an increase in tumour incidences. Toxic nephropathy was observed in rats that died within 20 wk (24).

The National Toxicology Program tested rats and mice via inhalation. Clear evidence of carcinogenicity in ♂ rats and ♂ and ♀ mice, some evidence of carcinogenicity in ♀ rats (25).

Intraperitoneal mouse (24 wk) 0, 80, 200 or 400 mg kg⁻¹ 3 × wk⁻¹ for up to 16 wk did not cause a significant increase in the number of lung tumours compared with controls (26).

Inhalation rat and mouse, 0, 200 or 400 ppm for rats, 0, 100 or 200 ppm for mice 6 hr day⁻¹ 5 days wk⁻¹ for 103 wk. The 400 ppm dose reduced survival in ♂ rats. Survival was reduced in all treated ♂ mice and among high-dose ♀ mice. Mononuclear cell leukaemia was associated with treated rats. Renal tubular cell karyomegaly occurred in both sexes of rats and renal tubular cell hyperplasia and neoplasms in ♂ rats. Dose-related increased incidences of hepatocellular neoplasms and renal tubular karyomegaly occurred in both sexes of mice (27).

Teratogenicity and reproductive effects

Inhalation rat, lowest toxic concentration 900 ppm for 7 hr day⁻¹ on days 7-13 of gestation (number of live births, metabolic effects and behavioural effects among offspring) (28).

Inhalation rat, lowest toxic concentration 1000 ppm for 24 hr day⁻¹ 14 days prior to mating through to day 22 of gestation (foetotoxicity and teratogenicity) (29).

Inhalation ♂ mouse, lowest toxic dose 500 ppm 7 hr day⁻¹ for 5 days (spermatogenesis) (30).

Metabolism and toxicokinetics

Slightly absorbed from the gastro-intestinal tract. Absorption is increased in the presence of alcohol, fats and oils. Absorbed via inhalation and through the skin. It is excreted unchanged in expired air (species unspecified) (31).

Mice excreted ~90% of inhaled dose of 1300 mg kg⁻¹, 70% in expired air, 20% in urine and <0.5% in faeces.

Metabolites identified in the urine were trichloroacetic acid (52% urinary metabolites), oxalic acid (11%) and traces of dichloroacetic acid. In contrast, only 2% of an oral dose of 1000 mg kg⁻¹ was found in the urine (32,33).

Irritancy

Dermal rabbit (24 hr) 810 mg caused severe irritation and 160 mg instilled into rabbit eye caused mild irritation (exposure unspecified) (34).

Dermal rabbit (24 hr) 500 mg caused mild irritation and 50 mg instilled into rabbit eye for 24 hr caused mild irritation (35).

Sensitisation

No sensitisation was observed in guinea pigs (36).

Skin sensitisation was reported in workers occupationally exposed (37).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA135, TA1537 with and without metabolic activation negative (38).

Saccharomyces cerevisiae gene conversion, homozygosis and reverse mutation negative (39).

Drosophila melanogaster sex-linked recessive lethal assay negative (40).

In vitro Chinese hamster ovary cells with and without metabolic activation sister chromatid exchanges and chromosomal aberrations negative (41).

In vitro primary rat hepatocytes unscheduled DNA synthesis negative (42).

In vitro mouse lymphoma L5178Y cells, tk⁺/tk⁻ forward mutation assay with and without metabolic activation negative (43).

In vivo human lymphocytes chromosomal aberrations negative (44).

In vivo rat liver foci induction, with diethylnitrosamine promotion, positive (45).

Other effects

Other adverse effects (human)

Dependence may follow habitual inhalation of small quantities of vapour. Coma, cardiac arrhythmias and death have followed sniffing of tetrachloroethylene (31).

Inhalation human (2 hr) lowest toxic concentration 280 ppm, central nervous system effects (46).

Oral child, LD_{Lo} 545 mg kg⁻¹ (47).

Narcotic at high concentrations. Defatting action on skin can lead to dermatitis (48).

General cohort and proportionate mortality studies have been made among laundry and dry-cleaning workers, who may have been exposed to other solvents, especially trichloroethylene and petroleum solvents. Excesses have been reported of lymphosarcomas, leukaemias and cancers of the skin, colon, lung and urogenital tract, although in one study, no excess of urogenital cancer was seen among workers exposed mainly to tetrachloroethylene (49-53). Some excess of lymphomas and cancers of the larynx and bladder was seen in a large cohort study of dry cleaners (54).

A familial cluster of chronic lymphocytic leukaemia has been related to dry cleaning (55).

A large case-control study of bladder cancer did not show any clear association with dry-cleaning (56).

In other case-control studies, dry-cleaning appeared to be a risk factor for pancreatic cancer and liver cancer (57-60).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (61).

WHO guideline value for drinking water 40 µg l⁻¹ (62).

Other comments

Detected in air, water and food samples, and in marine animal and human tissues (63,64).

Physical properties, uses, occurrence, analysis, carcinogenicity, mammalian toxicology and mutagenicity reviewed (63,65-69).

Environmental fate reviewed (64).

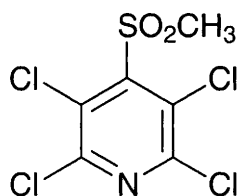
References

1. McCoy, G. D. et al *Carcinogenesis* 1990, 11(7), 1111-1117.
2. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, 63(3), 198-207.
3. Smith, A. D. et al *Arch. Environ. Contam. Toxicol.* 1991, 20, 94-102.
4. Konemann, W. H. *Quantitative Structure-Activity Relationships for Kinetics and Toxicity of Aquatic Pollutants and their Mixtures to Fish* 1987, Univ. Utrecht, Netherlands.

5. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
6. Denillers, J. et al *Chemosphere* 1987, **16**(6), 1149-1163.
7. Neely, W. B. et al *Environ. Sci. Technol.* 1974, **8**, 1113-1115.
8. Barrows, M. E. et al *Dynamic Exposure Hazards Assessment for Toxic Chemicals* 1980, 379-392, Ann Arbor Sci., MI, USA.
9. Bouwer, E. J. et al *Ground Water* 1984, **22**, 433-440.
10. Bouwer, E. J. et al *Appl. Environ. Microbiol.* 1983, **45**, 1286-1294.
11. Vogel, T. M. et al *Appl. Environ. Microbiol.* 1985, **49**, 1080-1083.
12. Mudder, T. I. *Am. Chem. Soc. Div. Environ. Chem. Conf. Kansas City* 1982, 52-53.
13. Lingh, H. B. et al *Atmos. Environ.* 1981, **15**, 601-612.
14. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
15. Schwartzboch, R. P. et al *Environ. Sci. Technol.* 1981, **15**, 1360-1367.
16. Chiou, C. T. et al *Science* 1979, **206**, 831-832.
17. *Am. Ind. Hyg. Assoc. J.* 1959, **20**, 364.
18. NTIS Report No. PB257-185 National Technical Information Service, Springfield, VA, USA.
19. *Toxicol. Appl. Pharmacol.* 1967, **10**, 119.
20. Klaasen, C. D. et al *Toxicol. Appl. Pharmacol.* 1966, **9**, 139-151.
21. *Quant. J. Pharm. Pharmacol.* 1934, **7**, 205.
22. Pegg, D. G. et al *Toxicol. Appl. Pharmacol.* 1978, **45**, 276-277.
23. *IARC Monograph* 1987, **Suppl. 7**, 355-356.
24. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-13, NIEHS, Research Triangle Park, NC, USA.
25. *National Toxicology Program Research and Testing Division* 1999, Report No. TR-311, NIEHS, Research Triangle Park, NC, USA.
26. Theiss, J. C. et al *Cancer Res.* 1977, **37**, 2717-2720.
27. Mennear, J. H. *Toxicol. Lett.* 1986, **31**(Suppl.), 16 (Abstract).
28. *Teratology* 1979, **19**, 41A.
29. *Abstr. of Papers. Soc. Toxicol. Ann. Meet.* 1980, **19**, 721.
30. NTIS Report No. PB82-185075 Natl. Tech. Inf. Ser., Springfield, VA, USA.
31. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
32. Yllner, S. *Nature (London)* 1961, **191**, 820.
33. Deviel, J. W. *Biochem. Pharmacol.* 1963, **12**, 795-802.
34. *J. Eur. Toxicol.* 1976, **9**, 171.
35. Marhold, J. V. *Prehled Prumyslove Toxikologie: Organické Latky* 1986, Prague, Czechoslovakia.
36. Rao, K. S. et al *Drug Chem. Toxicol.* 1981, **4**, 331-351.
37. Vail, J. T. *Arch. Dermatol.* 1974, **110**, 130.
38. Haworth, S. et al *Environ. Mol. Mutagen.* 1983, **5**(Suppl. 1), 3-142.
39. Callen, D. F. et al *Mutat. Res.* 1980, **77**, 55-63.
40. Velencia, R. et al *Environ. Mol. Mutagen.* 1985, **7**, 325-348.
41. Zeiger, E. et al *Environ. Mol. Mutagen.* 1990, **16**(Suppl. 18), 1-14.
42. Shimada, T. et al *Cell Biol. Toxicol.* 1985, **1**, 159-179.
43. McGregor, D. B. et al *Environ. Mol. Mutagen.* 1988, **12**(1), 85-154.
44. Ikeda, M. et al *Toxicol. Lett.* 1980, **5**, 251-256.
45. Milmen, H. A. et al *Ann. N. Y. Acad. Sci.* 1988, **534**, 521-530.
46. *AMA Arch. Ind. Hyg. Occup. Med.* 1952, **5**, 566.
47. *J. Toxicol. Clin. Toxicol.* 1985, **23**, 103.
48. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
49. Katz, R. M. et al *Am. J. Publ. Health* 1981, **71**, 305-307.
50. Blair, A. et al *Am. J. Publ. Health* 1979, **69**, 508-511.
51. Duh, R. W. et al *Am. J. Publ. Health* 1984, **74**, 1278-1280.
52. Kaplan, S. D. *Dry Cleaners Workers Exposed to Perchloroethylene. A Retrospective Cohort Study* 1980, NTIS, Springfield, VA, USA.
53. Brown, D. P. et al *J. Occup. Med.* 1987, **29**, 535-541.
54. Blair, A. et al *Med. Lav.* 1986, **77**, 82-83.
55. Blattner, W. A. et al *Ann. Intern. Med.* 1976, **84**, 554-557.
56. Smith, E. M. et al *J. Occup. Med.* 1985, **27**, 295-297.
57. Lin, R. S. et al *J. Am. Med. Assoc.* 1981, **245**, 147-152.
58. Stemhagen, A. et al *Am. J. Epidemiol.* 1983, **117**, 443-454.

59. Hardnell, L. et al *Br. J. Cancer* 1984, **50**, 389-397.
60. Hernberg, S. et al *Int. Arch. Occup. Environ. Health* 1984, **54**, 147-153.
61. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
62. *Guidelines for Drinking Water Quality* 2nd ed., 1993, **1**, WHO, Geneva, Switzerland.
63. *IARC Monograph* 1979, **20**, 491-513.
64. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1991, **2**, 418-429, Lewis Publishing, Chelsea, MI, USA.
65. HSE *Tetrachloroethylene. Toxicity Review* 17 1987, HMSO, London, UK.
66. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
67. *Environmental Health Criteria No. 31 Tetrachloroethylene* 1984, WHO, Geneva, Switzerland.
68. *Health and Safety Guide. Tetrachloroethylene* 1987, WHO, Geneva, Switzerland.
69. *Chemical Safety Data Sheets* 1989, **1**, The Royal Society of Chemistry, London, UK

T52 2,3,5,6-tetrachloro-4-(methylsulfonyl)pyridine



C₆H₃Cl₄NO₂S

Mol. Wt. 294.97

CAS Registry No. 13108-52-6

Synonyms methyl 2,3,5,6-tetrachloro-4-pyridyl sulfone

EINECS No. 236-035-5

RTECS No. UT 6160000

Uses Fungicide. Disinfectant.

Physical properties

M. Pt. 138-140°C

Occupational exposure

Supply classification harmful

Risk phrases Harmful in contact with skin and if swallowed – Irritating to the eyes – May cause sensitisation by skin contact (R21/22, R36, R43)

Safety phrases Keep out of reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – After contact with skin, wash immediately with plenty of water (S2, S26, S28)

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 770 mg kg⁻¹ (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (2).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (3).

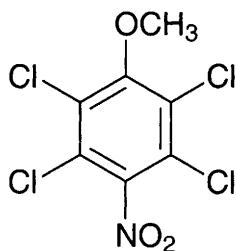
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (4).

References

1. *Nichidai Igaku Zasshi* 1981, **40**, 329.
2. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
3. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
4. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T53 2,3,5,6-tetrachloro-4-nitroanisole



$C_7H_3Cl_4NO_3$

Mol. Wt. 290.92

CAS Registry No. 2438-88-2

Synonyms 4-nitro-2,3,5,6-tetrachloroanisole; TCNA; 1,2,4,5-tetrachloro-3-methoxy-6-nitrobenzene; tetrachloroanisole

RTECS No. BZ 9625000

Uses Pesticide.

Physical properties

M. Pt. 101-105°C **Partition coefficient** $\log P_{ow}$ 3.9654 (1)

Solubility Organic solvents: acetone

Mammalian & avian toxicity

Acute data

LD_{50} oral rat 260 mg kg^{-1} (2).

Carcinogenicity and chronic effects

National Toxicology Program tested rats and mice via feed. Negative results were reported for ♂ and ♀ rats and mice (3).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (4,5). *In vitro* mouse lymphoma L5178Y cells, tk⁺/tk⁻ forward mutation assay positive (metabolic activation unspecified) (6).

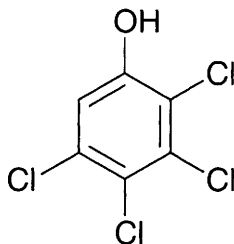
Legislation

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th Amendments) (7). Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (8). Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (9).

References

1. McCoy, G. D. et al *Carcinogenesis* 1990, **11**(7), 1111-1117.
2. *Ind. Hyg. Foundat. Am. Chem. Toxicol. Ser.* 1967, **6**, 1.
3. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-114, NIEHS, Research Triangle Park, NC, USA.
4. Klopman, G. et al *J. Comput. Chem.* 1988, **9**(3), 232-243.
5. Zeiger, E. et al *Environ. Mol. Mutagen.* 1992, **19**(Suppl. 2), 2-141.
6. McGregor, D. B. et al *Environ. Mol. Mutagen.* 1988, **12**(1), 85-154.
7. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
8. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
9. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T54 2,3,4,5-tetrachlorophenol



$\text{C}_6\text{H}_2\text{Cl}_4\text{O}$

Mol. Wt. 231.89

CAS Registry No. 4901-51-3

Synonyms 2,3,4,5-tetrachlorohydroxybenzene; tetrachlorophenol

EINECS No. 225-531-7

RTECS No. SM 9200000

Uses Fungicide. Organic synthesis.

Physical properties

M. Pt. 116-117°C (also given as 69-70°C) **B. Pt.** 164°C at 23 mmHg **Specific gravity** 1.6 at 60°C with respect to water at 4°C **Partition coefficient** log P_{ow} 4.21 (1)

Solubility Water: $<1 \text{ g l}^{-1}$ at 21°C. Organic solvents: acetone, diethyl ether, dimethyl sulfoxide, ethanol, light petroleum, ligroin

Occupational exposure

SE-LEVL 0.5 mg m^{-3}

SE-STEL 1.5 mg m^{-3}

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) guppy 1.1 mg l⁻¹ at pH 6.1 (2).

LC₅₀ (96 hr) fathead minnow 410 mg l⁻¹ flow-through bioassay (3).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 0.18 ppm Microtox test (4).

IC₅₀ (24 hr) *Daphnia magna* 1.7 mg l⁻¹ (5).

IC₅₀ (30 min) *Bacillus* sp. 4 mg l⁻¹ (6).

Environmental fate

Degradation studies

Degraded via dechlorination by *Rhodococcus chlorophenolicus* (7).

Virtually all 2,3,4,5-tetrachlorophenol disappeared from paddy soils (100 mg kg⁻¹ dry soil) after 4 wk incubation *in vitro* (8).

Adsorption and retention

Calculated soil sorption coefficient log K_{om} of 3.22 indicates that adsorption to soil and sediments would be significant (9).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 140, 400 mg kg⁻¹, respectively (10,11).

LD_{Lo} dermal rat 2000 mg kg⁻¹ (12).

LD₅₀ intraperitoneal mouse 97 mg kg⁻¹ (10).

Carcinogenicity and chronic effects

There is limited evidence for carcinogenicity of occupational exposure to chlorophenols to humans (13).

Metabolism and toxicokinetics

Trichloro-*p*-hydroquinone is formed in minor amounts. Of the 3 isomers, only 2,3,5,6-tetrachlorophenol is metabolised to a significant extent in rats (10).

60% of dose eliminated in the urine within 72 hr of intraperitoneal administration to rats (10).

Irritancy

Causes severe irritation to the eyes, skin, mucous membranes and upper respiratory tract (species unspecified) (14).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535 with and without metabolic activation negative (15).

In vitro Chinese hamster ovary and lung cells chromosomal aberrations with metabolic activation positive (16).

Other effects

Other adverse effects (human)

May be fatal if inhaled, swallowed or absorbed through the skin (14).

Legislation

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th Amendments) (17).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (18).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (19).

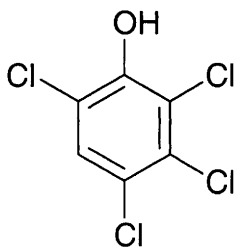
Other comments

Occurrence, environmental fate, mammalian toxicology and metabolism of chlorophenols reviewed (20,21).

References

1. Camilleri, P. et al *J. Chem. Soc. Perkin Trans. II* 1988, (9), 1699-1707.
2. Konemann, W. H. et al *Toxicology* 1981, **19**, 223-228.
3. Geiger, D. L. et al (Eds.) *Acute Toxicities of Organic Chemicals to Fathead Minnows* 1985, **2**(75), Univ. Wisconsin-Superior, USA.
4. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
5. Devillers, J. et al *Chemosphere* 1987, **16**(6), 1149-1163.
6. Lin, D. et al *Bull. Environ. Contam. Toxicol.* 1982, **29**, 130-136.
7. Apajalahti, J. H. A. et al *J. Bacteriol.* 1987, **169**(2), 675-681.
8. Ide, A. et al *Agric. Biol. Chem.* 1972, **26**(11), 1937-1944.
9. Sabljic, A. *Environ. Sci. Technol.* 1987, **21**(4), 358-366.
10. Ahlborg, U. G. et al *Arch. Toxicol.* 1978, **40**, 63-74.
11. *Proc. Int. Conf. Ind. Environ. Xenobiol. (Prague, 1980)* 1981, 309.
12. *Bull. Environ. Contam. Toxicol.* 1983, **31**, 680.
13. *IARC Monograph* 1986, **41**, 319-355.
14. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3248, Sigma-Aldrich, Milwaukee, WI, USA.
15. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-158.
16. Sofuni, T. et al *Mutat. Res.* 1990, **241**, 175-213.
17. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
18. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
19. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
20. *IPCS Environmental Health Criteria No. 93 Chlorophenols other than Pentachlorophenol* 1989, WHO, Geneva, Switzerland.
21. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T55 2,3,4,6-tetrachlorophenol



$C_6H_2Cl_4O$

Mol. Wt. 231.89

CAS Registry No. 58-90-2

Synonyms Dowicide b; TECP; 2,4,5,6-tetrachlorophenol; tetrachlorophenol

EINECS No. 200-402-8

RTECS No. SM 9275000

Uses Disinfectant. Fungicide. Manufacture of pesticides.

Physical properties

M. Pt. 69-70°C B. Pt. 164°C at 23 mmHg Specific gravity 1.6 at 60°C with respect to water at 4°C

Partition coefficient $\log P_{ow}$ 4.45 (1) Volatility v.p. 1 mmHg at 100°C

Solubility Water: <1 g l⁻¹ at 20°C. Organic solvents: acetone, benzene, chloroform, dimethyl sulfoxide, ethanol, ligroin

Occupational exposure

SE-LEVL 0.5 mg m⁻³

SE-STEL 1.5 mg m⁻³

UN No. 2020 HAZCHEM Code 2X Conveyance classification harmful substance

Supply classification toxic, dangerous for the environment

Risk phrases Toxic if swallowed – Irritating to eyes and skin – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R25, R36/38, R50/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – After contact with skin, wash immediately with plenty of water – Wear suitable gloves - In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S26, S28, S37, S45, S60, S61)

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) guppy, goldfish, brown trout 0.75-2.3 mg l⁻¹ (2-4).

Invertebrate toxicity

EC₅₀ (96 hr) *Selenastrum capricornutum*, *Chlorella vulgaris* 1.3, 10 ppm, respectively (4).

EC₅₀ (30 min) *Photobacterium phosphoreum* 1.27 ppm Microtox test (5).

Bioaccumulation

Bioconcentration factor for roach, pike, brown trout, goldfish 93-450 (2,6,7).

Environmental fate

Degradation studies

Degraded by bacteria in mixed soils at concentrations of 10-100 ppm. Other isomers were not degraded (8).

Degraded by *Rhodococcus chlorophenolicus* (9).

Virtually all 2,3,4,6-tetrachlorophenol disappeared from paddy soils (100 mg kg⁻¹ dry soil) after 4 wk incubation *in vitro* (10).

Adsorption and retention

Calculated soil sorption coefficient, log K_{om} of 3.32 indicates that adsorption to soil and sediments would be significant (11).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, guinea pig 140, 250 mg kg⁻¹, respectively (12,13).

LD₅₀ dermal rat, rabbit 250, 490 mg kg⁻¹, respectively (14,15).

LD_{Lo} subcutaneous rat 210 mg kg⁻¹ (15).

LD₅₀ intraperitoneal rat 130 mg kg⁻¹ (16).

Sub-acute and sub-chronic data

Gavage rat 0, 10, 50 or 100 mg kg⁻¹ day⁻¹ for 55 days caused histological changes in the liver, even though higher concentrations were found in the spleen and kidneys (17).

Carcinogenicity and chronic effects

There is limited evidence for carcinogenicity of occupational exposure to chlorophenols to humans (18).

Teratogenicity and reproductive effects

Gavage rat, 10 or 30 mg kg⁻¹ day⁻¹ on days 6-15 of gestation caused a delay in ossification of skull bones (19).

Metabolism and toxicokinetics

Toxic amounts may be absorbed through human skin (20).

Following intragastric administration of 100 mg kg⁻¹ day⁻¹ for 55 days to rats, tissue concentrations were 5.1 mg kg⁻¹ in the kidney, 3.2 mg kg⁻¹ in the spleen, 2.2 mg kg⁻¹ in the liver, 1.2 mg kg⁻¹ in the brain and 0.46 mg kg⁻¹ in the muscle (17).

Excreted in the urine exclusively as conjugates (21).

Trichloro-*p*-hydroquinone is formed in minor amounts in rats. Of the 3 isomers, only 2,3,5,6-tetrachlorophenol is metabolised to a significant extent (22).

Eliminated in the urine within 48 hr following intraperitoneal administration to rats (22).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535 with and without metabolic activation negative (23).

In vitro Chinese hamster V-79 cells without metabolic activation weakly positive (24).

In vitro Chinese hamster ovary and lung cells chromosome aberrations with metabolic activation positive (25).

Legislation

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th Amendments) (26).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (27).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (28).

Other comments

Detected in the urine of workers exposed in wood preservation processes and chlorophenol manufacture (18). Metabolite of lindane (20).

Occupational exposure to chlorophenols reviewed (18).

May contain polychlorinated-*p*-dioxins and polychlorodibenzofurans (18,20).

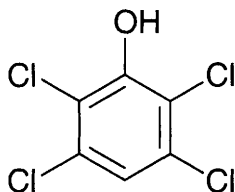
Physical properties, use, occurrence, environmental impact, mammalian toxicology and metabolism reviewed (20,29).

References

1. Camilleri, P. et al *J. Chem. Soc. Perkin Trans. II* 1988, (9), 1699-1707.
2. Hattula, M. L. et al *Bull. Environ. Contam. Toxicol.* 1981, **26** 295-298.
3. Kobayashi, K. et al *Bull. Jpn. Soc. Sci. Fish* 1979, **45**(2), 173-175.
4. Shigeoka, T. et al *Environ. Toxicol. Chem.* 1988, **7**, 847-854.
5. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
6. Prasivinta, J. et al *Chemosphere* 1985, **14**(5), 469-491.
7. Kobayashi, S. et al *J. Med. Soc. Toho. Univ. Jpn.* 1972, **19**, 356-362.
8. Kihohara, H. et al *J. Ferment. Bioeng.* 1989, **67**(5), 339-344.
9. Apajalahti, H. A. et al *J. Bacteriol.* 1987, **169**(2), 675-681.
10. Ide, A. et al *Agric. Biol. Chem.* 1972, **36**(11), 1937-1944.
11. Sabljic, A. *Environ. Sci. Technol.* 1987, **21**(4), 358-366.
12. *Ind. Med. Surgery* 1970, **39**, 56.
13. *Farm Chemicals Handbook* 1975, D200, Meister, Willoughby, OH, USA.
14. *Bull. Environ. Contam. Toxicol.* 1983, **31**, 680.
15. *Handbook Toxicol.* 1959, **5**, 129.
16. *Br. J. Pharmacol. Chemotherap.* 1958, **13**, 20.
17. Hattula, M. L. et al *Bull. Environ. Contam. Toxicol.* 1981, **26**, 795-800.
18. *IARC Monograph* 1986, **41**, 319-355.
19. Schwetz, B. A. et al *Toxicol. Appl. Pharmacol.* 1974, **28**, 146-150.
20. *IPCS Environmental Health Criteria No. 93 Chlorophenols other than Pentachlorophenol* 1989, WHO, Geneva, Switzerland.
21. Perkaui, K. et al *Proc. 26th Congr. Eur. Soc. Tox., Kuopio, Finland* 1985, 193.
22. Ahlborg, U. G. et al *Arch. Toxicol.* 1978, **40**, 63-74.
23. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-158.
24. Hattula, M. L. et al *Chemosphere* 1985, **14**, 1617-1625.
25. Sofuni, T. et al *Mutat. Res.* 1990, **241**, 175-213.

26. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
27. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
28. S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations 1991, HMSO, London, UK.
29. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T56 2,3,5,6-tetrachlorophenol



$C_6H_2Cl_4O$

Mol. Wt. 231.89

CAS Registry No. 935-95-5

Synonyms tetrachlorophenol

EINECS No. 213-310-8

RTECS No. SM 9450000

Occurrence Metabolite of lindane (1).

Physical properties

M. Pt. 114-116°C Partition coefficient $\log P_{ow}$ 3.88 (2)

Solubility Water: $<1 \text{ g l}^{-1}$ at 20°C. Organic solvents: acetone, benzene, dimethyl sulfoxide, ethanol, ligroin

Occupational exposure

SE-LEVL 0.5 mg m^{-3}

SE-STEL 1.5 mg m^{-3}

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) American flagfish 1.0-1.3 mg l^{-1} – flow-through bioassay (3).

LC₅₀ (96 hr) sheepshead minnow 1.9 mg l^{-1} (4).

LC₅₀ (24 hr) guppy 0.36-0.44 mg l^{-1} at pH 6.1, 2.3-3.9 at pH 7.8 (5).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 2.1-2.2 ppm, Microtox test (6).

EC₅₀ (24 hr) *Daphnia magna* 2.3 mg l^{-1} (7).

Bioaccumulation

Bioconcentration factor in sunfish, bass, catfish 72-8600 (8).

Environmental fate

Nitrification inhibition

IC₅₀ (25 day) *Nitrosomonas* sp. 1.3 mg l^{-1} (9).

Carbonaceous inhibition

IC₅₀ (5 day) aerobic heterotrophs isolated from activated sludge 1.5 mg l^{-1} (9).

Anaerobic effects

IC₅₀ (50 day) methanogenic bacterial culture 0.13 mg l⁻¹ (9).

Degradation studies

Degraded via dechlorination by *Flavobacterium* sp. acclimated to pentachlorophenol and by *Rhodococcus chlorophenolicus* (10,11).

Virtually all 2,3,5,6-tetrachlorophenol disappeared from paddy soils (100 mg kg⁻¹ soil) after 4 wk incubation *in vitro* (12).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 110 mg kg⁻¹ (13).

LD_{Lo} dermal rat 2000 mg kg⁻¹ (14).

LD_{Lo} intraperitoneal mouse 500 mg kg⁻¹ (15).

Carcinogenicity and chronic effects

There is limited evidence for carcinogenicity of occupational exposure to chlorophenols to humans (16).

Metabolism and toxicokinetics

Absorbed through rat skin (17).

Of the 3 isomers, only 2,3,5,6-tetrachlorophenol is metabolised to a significant extent in rats. 35% of 10 mg kg⁻¹ intraperitoneal dose was metabolised to tetrachloro-*p*-hydroquinone (13).

Eliminated in the urine within 24 hr, following intraperitoneal administration to rats (14).

Irritancy

Causes severe irritation to the skin, eyes, mucous membranes and upper respiratory tract (species unspecified) (18).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535 with and without metabolic activation negative (19).

In vitro Chinese hamster ovary and lung cells chromosomal aberrations with metabolic activation positive (20).

Other effects

Other adverse effects (human)

May be fatal if inhaled, swallowed or absorbed through the skin (18).

Legislation

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th Amendments) (21).

Other comments

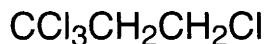
Physical properties, occurrence, environmental impact, mammalian toxicology and metabolism reviewed (1,22).

References

1. IPCS Environmental Health Criteria No. 93 Chlorophenols other than Pentachlorophenol 1989, WHO, Geneva, Switzerland.
2. Camilleri, P. et al *J. Chem. Soc. Perkin Trans. II* 1988, (9), 1699-1707.
3. Smith, A. D. et al *Arch. Environ. Contam. Toxicol.* 1981, **27**, 596-604.
4. Heitmüller, P. T. et al *Bull. Environ. Contam. Toxicol.* 1982, **29**, 130-136.
5. Konemann, W. H. et al *Toxicology* 1981, **19**, 223-228.
6. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
7. Devillers, J. et al *Chemosphere* 1987, **16**(6), 1149-1163.
8. Pierce, R. H. et al in *Pentachlorophenol. Chemistry, Pharmacology and Environmental Toxicology* Rao, K. R. (Ed.) 1978, 41-52, Plenum Press, New York, NY, USA.
9. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, **63**(3), 198-207.

10. Steient, J. G. et al *Appl. Environ. Microbiol.* 1987, **53**(5), 907-910.
11. Apajalahti, J. H. A. et al *J. Bacteriol.* 1987, **169**(2), 675-681.
12. Ide, A. et al *Agric. Biol. Chem.* 1972, **36**(11), 1937-1944.
13. Ahlborg, U. G. et al *Arch. Toxicol.* 1978, **40**, 63-74.
14. *Bull. Environ. Contam. Toxicol.* 1978, **40**, 63.
15. *Summary Table of Biological Tests* 1955, **7**, 788.
16. *IARC Monograph* 1986, **41**, 319-355.
17. Shen, S. Y. et al *Bull. Environ. Contam. Toxicol.* 1983, **31**, 680-685.
18. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3249, Sigma-Aldrich, Milwaukee, WI, USA.
19. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-158.
20. Sofuni, T. et al *Mutat. Res.* 1990, **241**, 175-213.
21. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
22. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T57 1,1,1,3-tetrachloropropane



$\text{C}_3\text{H}_4\text{Cl}_4$

Mol. Wt. 181.88

CAS Registry No. 1070-78-6

EINECS No. 213-981-7

RTECS No. TZ 7000000

Physical properties

B. Pt. 159°C Specific gravity 1.446 at 25°C with respect to water at 4°C

Solubility Organic solvents: benzene, chloroform, diethyl ether, ethanol

Mammalian & avian toxicity

Acute data

LD_{Lo} oral rat 1600 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

Inhalation rat (6 hr day⁻¹, 5 days wk⁻¹, for 90 days) 0, 25, 75 or 225 ppm. No significant differences were observed in body weight or food consumption; however, in the 225 ppm group liver and heart lesions were observed. The liver lesions were resolved by a 28-day recovery period, however the heart lesions remained in ♂ rats (2).

References

1. *Gig. Sanit.* 1962, **27**, 3.
2. Kolesar, G. B. et al *Fundam. Appl. Toxicol.* 1995, **25**(1), 52-59

T58 1,2,2,3-tetrachloropropane $\text{C}_3\text{H}_4\text{Cl}_4$

Mol. Wt. 181.88

CAS Registry No. 13116-53-5

EINECS No. 236-043-9

RTECS No. TZ 7000100

Physical properties

B. Pt. 165.5°C Specific gravity 1.500 at 18°C with respect to water at 4°C Volatility v.den. 6.28
Solubility Organic solvents: chloroform, diethyl ether, ethanol

Environmental fate**Abiotic removal**Evaporation $t_{1/2}$ 17 min for initial concentration of 1 ppm at 25°C (1).**Mammalian & avian toxicity****Sub-acute and sub-chronic data**Inhalation rat 0, 100, 300, 600 or 900 ppm for 6 hr day⁻¹, 5 days wk⁻¹ for 4 wk. Deaths occurred at 600 ppm.

Reduced body weights were seen in ♂ rats at all dose levels (2).

Inhalation rat 0-50 ppm for 6 hr day⁻¹ 5 days wk⁻¹ for 13 wk. Liver weights were increased at ≥5 ppm in ♂ rats.

Degenerative changes in the liver were also seen (2).

Teratogenicity and reproductive effectsInhalation rat 0, 5 or 15 ppm for 6 hr day⁻¹ 5 days wk⁻¹ for a pre-mating, mating or gestation period. Mating performance was poor in all exposed ♂ and in high-dose ♀ rats. No teratogenic effects were reported (2).**Irritancy**

Vapour inhalation caused irritation of mucosal tissue in rats (2).

References

1. Wendell, L. et al *Environ. Sci. Technol.* 1975, 9(9).
2. Johansson, F. R. et al *J. Toxicol. Environ. Health* 1988, 25(3), 317-328

T59 1,1,2,3-tetrachloropropene $\text{C}_3\text{H}_2\text{Cl}_4$

Mol. Wt. 179.86

CAS Registry No. 10436-39-2

Synonyms tetrachloropropene

EINECS No. 233-920-8

RTECS No. UD 1925000

Physical properties

B. Pt. 167-167.5°C Specific gravity 1.550 at 25°C with respect to water at 4°C

Solubility Organic solvents: benzene, chloroform

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 350, 800 mg kg⁻¹, respectively (1,2).

LC_{Lo} (4 hr) inhalation rat 250 ppm (2).

LD₅₀ dermal rabbit 400 mg kg⁻¹ (2).

Sub-acute and sub-chronic data

Gavage rat 0-300 mg kg⁻¹ day⁻¹ for 4 wk. 0/5 ♂ and 1/5 ♀ rats died. A dose-related reduction in food intake and mean body weight was observed. Treatment-related necrotic/degenerative lesions of the liver were seen in high-dose animals (3).

Inhalation rat 0, 1, 5 or 15 ppm for 6 hr day⁻¹ 5 days wk⁻¹ for 13 wk caused no clinical signs of toxicity or irritation (4).

Teratogenicity and reproductive effects

Inhalation rat 0, 1 or 5 ppm for 6 hr day⁻¹ 5 days wk⁻¹ for a 10 wk pre-mating period, a mating period, and the first 14 days of gestation (♀ only). Mating, pregnancy and fertility were comparable among all groups. No foetotoxic or teratogenic effects were observed (4).

Genotoxicity

Salmonella typhimurium TA1535 with metabolic activation fluctuation test positive (5).

Saccharomyces cerevisiae D7, XU185-14C without metabolic activation positive (6).

Escherichia coli WP2 fluctuation test weakly positive (5).

In vitro Chinese hamster ovary cells chromosomal aberrations with and without metabolic activation positive, sister chromatid exchanges without metabolic activation positive (5).

Other comments

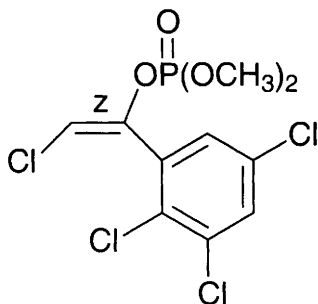
In chlorinated pulp mill effluents (5).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (7).

References

1. *Gig. Sanit.* 1978, **43**(4), 15.
2. *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 470.
3. Johannson, F. R. et al *Toxicol. Lett.* 1991, **57**(3), 347-352.
4. Johannson, F. R. et al *J. Toxicol. Environ. Health* 1991, **33**(3), 291-302.
5. Ellerton, J. A. et al *Can. J. Genet. Cytol.* 1981, **23**, 17-25.
6. Nestmann, E. R. et al *Mutat. Res.* 1983, **119**, 273-280.
7. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T60 tetrachlorvinphos



$C_{10}H_9Cl_4O_4P$

Mol. Wt. 365.96

CAS Registry No. 22248-79-9

Synonyms (Z)-2-chloro-1-(2,4,5-trichlorophenyl)vinyl dimethyl phosphate; phosphoric acid, 2-chloro-1-(2,4,5-trichlorophenyl)ethenyl dimethyl ester, (Z)-; CVMP; Appex; Debantic; Gardcide; Gardona; Rabon; Ridect

EINECS No. 244-865-4

RTECS No. TB 9100000

Uses Organophosphate insecticide.

Physical properties

M. Pt. 94-97°C **Partition coefficient** $\log P_{ow}$ 3.7 (1) **Volatility** v.p. 4.2×10^{-8} mmHg at 20°C
Solubility Water: 11 mg l⁻¹ at 20°C. Organic solvents: acetone, chloroform, dichloromethane, xylene

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) carp, rainbow trout, bluegill sunfish, channel catfish 0.36-6.0 mg l⁻¹ (2,3).

Invertebrate toxicity

LC₅₀ *Pieris brassicae* caterpillar ~80 mg l⁻¹ (4).

EC₅₀ (5 days) *Spinalina plantensis* 10 mg l⁻¹ at 25-28°C, pH 9.6-10.6 (5).

Toxic to bees (6).

Bioaccumulation

No or low bioaccumulation (5).

Environmental fate

Degradation studies

Primary route of dissipation is biotic degradation (7).

Abiotic removal

Hydrolysis $t_{1/2}$ 3600 hr at pH 5.75; 2400 hr at pH 6.5; 1100 hr at pH 7.4; 314 hr at pH 8.0; 60 hr at pH 9.0 (8).

Adsorption and retention

When applied to soil at 1.5 kg ha⁻¹ residues persisted for 60 days and were leached beyond a depth of 15 cm (9).

In the environment, tetrachlorvinphos is not persistent; its mobility increases as soil texture becomes coarser and the organic matter content decreases (7).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird, starling 100, >100 mg kg⁻¹, respectively (10).

LD₅₀ Chukar partridges and mallard ducks >2000 mg kg⁻¹; for various other birds 1500-2600 mg kg⁻¹ (6).

LC₅₀ (4 hr) inhalation mouse, cat, rabbit >290 mg m⁻³ (11).

LD₅₀ oral rat 480 mg kg⁻¹ (12).

LD₅₀ oral mouse 1380 mg kg⁻¹ (13).

LD₅₀ oral guinea pig 1600 mg kg⁻¹ (13).

LD₅₀ dermal rat 1500 mg kg⁻¹ (12).

LD₅₀ dermal rabbit 2500 mg kg⁻¹ (14).

LD₅₀ intraperitoneal rat, mouse 1200, 1500 mg kg⁻¹, respectively (15).

Sub-acute and sub-chronic data

Oral rat 10, 100 or 1000 mg kg⁻¹ day⁻¹ for 28 days caused a dose-related inhibition of serum cholinesterase and erythrocyte acetylcholinesterase activities. 1000 mg kg⁻¹ caused some fatalities among ♀ rats, and a reduced body weight gain in ♂ rats. The weights of adrenal gland, liver, kidney and thyroid were increased. The adrenal lesions were characterised by vacuolation and swelling of the cortex cells. The hepatic lesions consisted of vacuolation and necrosis of hepatocytes. The renal lesions consisted of regeneration and necrosis of tubular epithelial cells (16).

Dermal rat 0.08-2.0 mg cm⁻² day⁻¹ 5 day wk⁻¹ for 12 wk caused no systemic or topical effects (17).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (18).

Oral rat, mouse (2 yr) 750 or 3000 ppm diet for 1 yr caused a marked inhibition of cholinesterase activities. No necrotoxicity, teratogenicity or mutagenicity observed (13).

Of 100 mice fed diets containing 8 or 16 g kg⁻¹ for 80 wk, 36/50 of the low-dose group and 40/50 of the high-dose group developed hepatocellular carcinomas. The combined incidences of neoplastic nodules and hepatocellular carcinomas in the low-dose and high-dose ♀ were 19/49 and 11/47, respectively. In a parallel study in 100 rats, low-dose groups were fed 8 g kg⁻¹ for the first 5 wk then 4 g kg⁻¹ for 75 wk, and the high-dose groups 16 g kg⁻¹ and 8 g kg⁻¹, respectively. There was a dose-related incidence of C-cell adenoma and hyperplasia of the thyroid and adrenal cortical adenomas in ♀ rats (19).

Oral administration of doses ≤2 g kg⁻¹ did not induce a significant incidence of tumours in rats (duration unspecified) (12).

Teratogenicity and reproductive effects

Oral rat, mouse no teratogenic effects were observed in animals administered ≤3 g kg⁻¹ for 1 yr (administration procedures unspecified) (13).

Metabolism and toxicokinetics

Following oral administration of radiolabelled substance, 44-78% was eliminated in the urine within 24 hr, and 4-15% in the following 24 hr. 16.5% of the radiolabel was eliminated in the faeces and 0.5% in the expired air. In dogs, 92% was excreted in the urine and faeces within 4 days. The compound was completely metabolised in rats and dogs. Metabolites identified (percentages in rat and dog urine, respectively) were:

2,4,5-trichlorophenylethanedial glucuronamide (8 and 12%), [1-(2,4,5-trichlorophenyl)ethyl-β-D-glucopyranoside]-uronic acid (35 and 0%), 2,4,5-trichloromandelic acid (24 and 12%), 2-chloro-1-(2,4,5-trichlorophenyl)vinyl methyl hydrogen phosphate (4 and 46%), 2,4,5-trichlorophenylethanedial (2 and 4%), and 1-(2,4,5-trichlorophenyl)-ethanol (2 and 0%) (20).

No significant residues of tetrachlorvinphos and its metabolites were found in milk or tissues of exposed mammals (6).

Sensitisation

Patch tests in human subjects were negative in normal and hypersensitive subjects (17).

Genotoxicity

- Salmonella typhimurium* TA98, TA100 with and without metabolic activation negative (21).
Escherichia coli WP2, WP2 *trp* without metabolic activation negative (22).
Aspergillus nidulans induction of gene cross-over and non-disjunction positive (23).
In vitro human lymphocytes, chromosomal aberrations positive (24).
In vitro EUE human embryo fibroblasts, unscheduled DNA synthesis positive (25).
In vivo chicken bone marrow, DNA formation was inhibited (26).
In vivo mouse bone marrow, chromosomal aberrations negative (27).

Other effects

Other adverse effects (human)

Repeated doses of 15 mg day⁻¹ to human volunteers were reported to have no effect on plasma or red-cell cholinesterase activities (28).

Any other adverse effects

Induced hepatic microsomal enzymes in rats (details unspecified) (29).
Intraperitoneal rat, single dose of 500 mg kg⁻¹ depressed cholinesterase activity and reduced uptake of iodine by the thyroid glands (30).

Legislation

- Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (31).
Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (32).
The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (33).
WHO Toxicity Class Table 5 (34).
EPA Toxicity Class III (formulation) (6).
EC maximum residue levels: fruit 2 ppm, vegetables 0.5 ppm (35).

Other comments

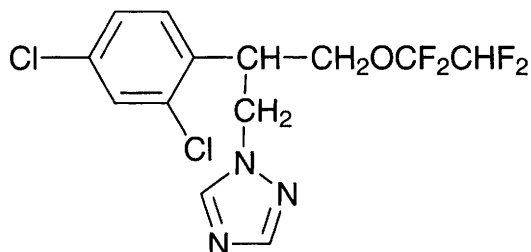
- Residues have been detected on fruits and foodstuffs.
No potentially toxic materials were detected among the identified degradation products (36).

References

1. McCoy, G. D. et al *Carcinogenesis* 1990, **11**(7), 1111-1117.
2. *Handbook of Acute Toxicity of Chemicals to Fish and Aquatic Invertebrates* 1980, 85, Resource Publ. 187, US EPA Fish and Wildlife Service, Washington, DC, USA.
3. Verkhovskii, A. P. et al *Byul. Vses. Inst. Eksp. Vet.* 1981, **41**, 45-49 (Russ.) (*Chem. Abstr.* **98**, 174420a).
4. Norozhilov, K. V. et al *Khim. Selsk. Kyo* 1977, **15**(4), 73-76 (Russ.) (*Chem. Abstr.* **87**, 17273k).
5. *JETOC Newsl.* 1987, **5**, 20-23, Japan Chemical Industry Ecology-Toxicology and Information Centre, Tokyo, Japan.
6. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
7. *Prevention, Pesticides and Toxic Substances (7508W)* September 1995, United States Environmental Protection Agency, EPA 738-R-95-036.
8. Akthar, M. H. et al *J. Agric. Food Chem.* 1977, **25**(4), 848-851.
9. Agnihotri, N. P. et al *Indian J. Agric. Chem.* 1981, **14**(1-2), 27-31.
10. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**(3), 355-382.
11. *Gig. Tr. Prof. Zabol.* 1975, **19**(4), 50.
12. Walker, A. I. T. et al *Pestic. Sci.* 1972, **3**, 517-525.
13. Wang, R. et al *Zhonghua Yufangyixue Zashi* 1987, **21**(2), 65-67.
14. Whetstone, R. R. et al *J. Agric. Food Chem.* 1966, **14**, 352-356.
15. Nishimura, M. et al *Jpn. J. Ind. Health* 1974, **16**, 523-530.
16. Ogawa, Y. et al *Eisei Shikensho Hokoku* 1990, **108**, 45-51, (Japan.) (*Chem. Abstr.* **114**, 201411f).
17. Huang, S. et al *Wuhan Yixueyuan Xuebao* 1983, **12**(1), 26-28.

18. IARC Monograph 1987, **Suppl.** 7, 56.
19. Bioassay of Tetrachlorovinphos for Possible Carcinogenicity 1978, 78-33, Natl. Cancer Inst. Tech. Report Series No. 33, NIEHS, Research Triangle Park, NC, USA.
20. Akintrwa, D. A. A. et al *J. Agric. Food Chem.* 1967, **15**, 632-637.
21. Bartsch, H. et al *Mutat. Res.* 1980, **76**(1), 1-50.
22. Nagy, Z. et al *Acta Microbiol. Acad. Sci. Hung.* 1975, **22**, 309-314.
23. Vallini, G. et al *Environ. Pollut. Ser. A.* 1983, **30**(1), 39-58.
24. Kurinnii, A. I. et al *Genetika* 1977, **13**, 337-339.
25. Berigni, R. et al *Mutat. Res.* 1980, **74**, 217.
26. Rusov, C. et al *Hrana Ishrama* 1988, **29**(4), 211-213, (Serbo-Croat.) (*Chem. Abstr.* **113**, 14769q).
27. Kurinnii, A. I. et al *Genetika* 1975, **11**, 64-69.
28. Rider, J. A. et al *Fed. Proc.* 1969, **28**, 479.
29. Jiang, Q. et al *Weishang Dulixue Zazhi* 1989, **3**(4), 196-198, (Ch.) (*Chem. Abstr.* **113**, 127865t).
30. Bojadziev, S. B. et al *Agressologie* 1975, **16**, 67-72.
31. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
32. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
33. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
34. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.2.
35. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
36. Farghaly, M. et al *Isot. Radiat. Res.* 1986, **18**(2), 131-137 (Eng.) (*Chem. Abstr.* **107**, 95475g)

T61 tetraconazole



$C_{13}H_{11}Cl_2F_4N_3O$

Mol. Wt. 372.15

CAS Registry No. 112281-77-3

Synonyms (RS)-2-(2,4-dichlorophenyl)-3-(1H-1,2,4-triazol-1-yl)propyl 1,1,2,2-tetrafluoroethyl ether;
(±)-1-[2-(2,4-dichlorophenyl)-3-(1,1,2,2-tetrafluoroethoxy)propyl]-1H-1,2,4-triazole

Uses Fungicide used in the control of powdery mildew, brown rust, *Septoria*, and *Rhynchosporium* on cereals; powdery mildew and scab on apples; powdery mildew on vines and cucumbers; powdery mildew and beet leaf spot on sugar beet; and powdery mildew and rust on vegetables (1).

Physical properties

M. Pt. 6°C (pour point) **B. Pt.** 240°C (decomp.) **Specific gravity** 1.432 at 20°C

Partition coefficient $\log P_{ow}$ 3.56 at 20°C **Volatility** v.p. 0.18 mPa

Solubility Water: 156 mg/l at pH 7 and 20°C. Organic solvents: acetone, 1,2-dichloroethane, methanol

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) rainbow trout, bluegill sunfish 4.8, 4.0 mg l⁻¹, respectively (1).

Invertebrate toxicity

LD₅₀ contact bee >100 µg bee⁻¹ (1).

LC₅₀ (48 hr) *Daphnia* 3.0 mg l⁻¹ (1).

Environmental fate

Adsorption and retention

No leaching occurs in standard soils. K_{oc} 531-1922 in four soil types (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral ♂ rats 1250, ♀ rats 1031 mg kg⁻¹ (1).

LC₅₀ inhalation (4 hr) rat >3.66 mg l⁻¹ (1).

LD₅₀ dermal rat >2000 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

LC₅₀ (8 day) bobwhite quail, mallard ducks 650, 422 mg kg⁻¹ in diet, respectively (1).

Carcinogenicity and chronic effects

Oral rat (2 yr) no-observed-adverse-effect level 80 ppm in diet (1).

Metabolism and toxicokinetics

Readily absorbed, metabolised and excreted in mammals, with no significant retention in tissues. In the rat the main metabolite identified in urine is 1,2,4-triazole (1).

Genotoxicity

Non-mutagenic in Ames test (1).

Legislation

WHO Toxicity Class II (2).

Limited under EC Directive on Drinking Water Quality 80/788/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (3).

Included in Schedules 5 and 6 (Release into Water and Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (4).

Other comments

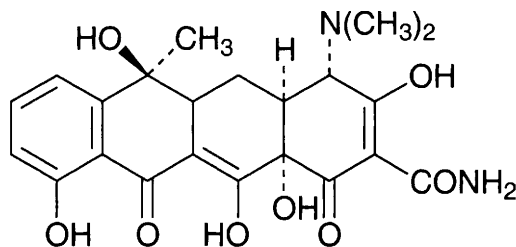
Tetraconazole is an inhibitor of P450-based enzymes and in maize seedlings acts as a potential activator of plant defence responses to abiotic and biotic challenges (5).

Extensively metabolised in plants. Tetraconazole acid, tetraconazole alcohol, triazolylalanine and triazolylacetic acid have been identified as metabolites (1).

References

1. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
2. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
4. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
5. Ronchi, A. et al *Plant Sci. (Shannon, Irel.)* 1997, **130**(1), 51-62

T62 tetracycline



C₂₂H₂₄N₂O₈

Mol. Wt. 444.44

CAS Registry No. 60-54-8

Synonyms 4-(dimethylamino)-1,4,4 α ,5,5 α ,6,11,12 α -octahydro-3,6,10,12,12 α -pentahydroxy-6-methyl-1,11-dioxo-2-naphthacene-carboxamide; deschlorobiomycin; tsiklomitsin; Abricycline; Cyclomycin; Polycycline; Steclin; Veracin; Tetrafil; Tetrabon

EINECS No. 200-481-9

RTECS No. QI 8750000

Uses Anti-amoebic. Antibacterial. Used in the treatment of fish diseases.

Physical properties

M. Pt. 170-175°C (decomp.)

Solubility Water: 1.7 mg l⁻¹ at 28°C. Organic solvents: methanol

Ecotoxicity

Fish toxicity

Pharmacokinetics and bioavailability in channel catfish were determined by administering 4 mg kg⁻¹ hydrochloride (body weight, intravascularly). Plasma t_{1/2} were established at 1.3 and 16.5 hr for the distribution and elimination phases, respectively. Tetracycline concentrated in both the hepatobiliary and urinary compartments. There were no significant concentrations in edible flesh. 72% was bound to plasma protein at both 4 and 24 hr after administration (1).

Environmental fate

Abiotic removal

Irradiation of the phototoxic antibiotic tetracycline in acetonitrile yielded 50% lumitetracycline; 70% was obtained from tetracycline hydrochloride in aqueous media (2).

Adsorption and retention

Interaction with model clay adsorbents was studied as a function of suspension pH, ionic strength and adsorbate concentration. The model clay adsorbents were the sodium, calcium, and dodecyltrimethylammonium forms of bentonite and a tannic-treated bentonite. Adsorption capacity decreased in the order: tannic acid-clay > Ca-clay > Na-clay > dodecyltrimethylammonium-clay. Adsorption decreased with increased ionic strength and pH (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat, guinea pig 678, 808, 1875 mg kg⁻¹, respectively (4-6).

LD₅₀ intravenous rat, mouse 130, 160 mg kg⁻¹, respectively (7,8).

LD₅₀ intraperitoneal mouse, rat 125, 310 mg kg⁻¹, respectively (9,10).

Carcinogenicity and chronic effects

Oral rats, mice (2 yr) 0, 12,500 or 25,000 ppm (hydrochloride) (equivalent to 20 to 140 × the human therapeutic dose). Dose-related increased survival in ♀ rats and ♂ mice. Basophilic cytoplasmic and clear cell changes observed in livers of ♂ rats, but no carcinogenic effects (11).

Teratogenicity and reproductive effects

In women receiving a single 1000 mg insertion of tetracycline or three 200 mg insertions, respectively, for nonsurgical ♀ sterilisation, tetracycline was unsatisfactory, with a 34 and 58% failure rate (12).

Developmental toxicity studies in humans, tetracycline caused brown staining of deciduous teeth (second- or third-trimester exposure only) (13).

Intraperitoneal pika (8-18 day gestation) 0, 5, 25, 50, 75 mg kg⁻¹ caused skeletal malformations in foetuses.

Intraperitoneal rat (14-15 day gestation) 85 mg kg⁻¹ was lethal. Subcutaneous mouse (10-18 day gestation) 250 mg kg⁻¹ caused growth suppression and lethality (postnatally). Intraperitoneal intravenous rabbit (day 9 gestation) single dose 30-230 mg kg⁻¹ no structural or functional abnormalities observed (14).

Forelimb buds of day 14 rat foetuses were transplanted subcutaneously into athymic mice. On the 7th, 9th and 11th day after grafting mice were administered 1500 or 3000 mg kg⁻¹ in 0.5% carboxymethyl-cellulose intraperitoneally. No inhibition of growth occurred (15).

Metabolism and toxicokinetics

The duration of absorption from the gastro-intestinal tract was 3 hr (species unspecified) (16).

Intravenous sheep single dose 5 mg tetracycline kg⁻¹ peak concentration observed 5 min after infusion.

Tetracycline achieved high lymph concentrations (17).

Tetracyclines are known to be deposited in the bone of mammals (18).

Bioavailability in humans is 77% (18).

Incompletely absorbed from the gastro-intestinal tract, bioavailability in humans 60-80%. Peak plasma concentrations occur 1-3 hr after ingestion. Elimination is via urine and faeces (19).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (hydrochloride) (20,21).

Escherichia coli SOS chromotest without metabolic activation, recombinogenic effects positive (22).

In vitro Syrian hamster embryo cells, sister chromatid exchanges, unscheduled DNA synthesis and morphological transformation negative (23).

In vitro Chinese hamster ovary cells with and without metabolic activation negative (hydrochloride) (24).

In vivo mouse lymphoma L5178Y tk⁺/tk⁻ with and without metabolic activation equivocal (25).

Other effects

Other adverse effects (human)

Pharmaceutical industry workers in Cuba, occupationally exposed to tetracycline powder had blood plasma levels similar to therapeutic dosing (~50 × the acceptable levels). The hepatic system was most damaged by the drug. One worker presented a transitory myopia (26).

In humans, adverse effects include gastro-intestinal disturbance, renal dysfunction (mainly in existing renal impairment), hepatotoxicity, raised intracranial pressure, skin reactions and superinfection (19).

Any other adverse effects

Groups of cockerels were treated with daily (unspecified) doses of tetracycline or heat-degraded tetracycline for 6 days. Histopathological examination revealed degenerative changes in the liver and kidneys of treated birds. Serum uric acid concentrations were elevated but no alteration was observed in alanine aminotransferase activity and creatine concentration (27).

In vitro Chinese hamster, lung cells concentration >300 µg ml⁻¹ for 24-48 hr inhibited growth; 1000 µg ml⁻¹ for 6-24 hr caused 30-100% inhibition of cell survival, 100-1000 µg ml⁻¹ inhibited DNA, RNA and protein synthesis in a concentration-dependent manner (28).

Legislation

Recommended withdrawal time (U.S.) in farmed channel catfish treated with oxytetracycline is 21 days before marketing, with regard to human food safety (29).

Other comments

Metabolism, pharmacokinetics, toxicology and side-effects reviewed (30-32).

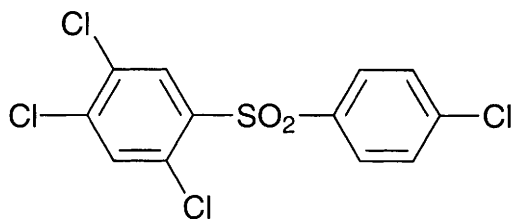
Human health effects and associated risks with the use of tetracycline at sub-therapeutic concentrations in animal feed reviewed (33).

Often administered as the hydrochloride CAS RN 64-75-5.

References

1. Plakas, S. M. et al *Xenobiotica* 1988, **18**(1), 83-93.
2. Drexel, R. E. et al *J. Org. Chem.* 1990, **55**(8), 2471-2478.
3. Sithole, B. B. et al *Water, Air, Soil Pollut.* 1987, **32**(3-4), 303-314.
4. *Am. J. Trop. Med. Hyg.* 1953, **2**, 254.
5. Goldenthal, E. I. *Toxicol. Appl. Pharmacol.* 1971, **18**, 185.
6. Izmerov, N. F. *Toxicometric Parameters of Industrial Toxic Chemicals Under Single Exposure* 1982, **109**, CIP, Moscow, USSR.
7. *Antibiot. Chemother.* 1954, **4**, 411.
8. *Farmaco, Ed. Sci.* 1955, **10**, 346.
9. *Takeda Kenkyusho Nempo. Ann. Rep. Takeda Res. Lab.* 1955, **14**, 60.
10. *Drugs in Japan. Ethical Drugs* 6th ed., 1982, 493, Tokyo, Japan.
11. Dietz, D. D. et al *Fundam. Appl. Toxicol.* 1991, **17**(2), 335-346.
12. Mullick, B. et al *Adv. Contracept.* 1987, **3**(3), 245-254.
13. Jelovsek, F. R. et al *Obstet. Gynecol.* 1989, **74**(4), 624-636.
14. Nishimura, H. et al *Exp. Anim.* 1986, **35**(4), 387-408.
15. Shiota, K. et al *Reprod. Toxicol.* 1990, **4**, 95-103.
16. Groening, R. et al *Pharm. Acta Helv.* 1989, **64**(3), 71-75 (Ger.) (*Chem. Abstr.* **110**, 185318r).
17. Cohen, S. H. *Diagn. Microbiol. Infect. Dis.* 1987, **6**(1), 53-58.
18. Gilman, A. G. (Ed.) *The Pharmacological Basis of Therapeutics* 1985, 1170-1198, MacMillan, New York, NY, USA.
19. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
20. Zeiger, E. *Environ. Mol. Mutagen.* 1990, **16**(Suppl. 18), 32-54.
21. Zeiger, E. *Environ. Mutagen.* 1987, **9**(Suppl. 9), 1-109.
22. Tenenbaum, L. et al *Mutat. Res.* 1988, **203**, 415-426.
23. Suzuki, H. *Shigaku* 1987, **74**(6), 1385-1403 (Japan.) (*Chem. Abstr.* **107**, 822x).
24. Anderson, B. E. et al *Environ. Mol. Mutagen.* 1990, **16**(Suppl. 18), 55-137.
25. Myhr, B. et al *Environ. Mol. Mutagen.* 1990, **16**(Suppl. 18), 138-167.
26. Bueno-Santiso, E. et al *Rev. Cubana Hig. Epidemiol.* 1988, **26**(1), 5-14 (Span.) (*Chem. Abstr.* **109**, 236115m).
27. Berkhin, E. B. et al *Farmakol. Toksikol. (Moscow)* 1987, **50**(5), 37-38 (Russ.) (*Chem. Abstr.* **107**, 168281u).
28. Sato, M. *Shigaku* 1988, **76**(5), 898-910 (Japan.) (*Chem. Abstr.* **110**, 88082b).
29. Schnick, R. A. et al *Progressive Fish-Culturist* 1986, **48**, 1-17.
30. Kobayashi, Y. *Pharma. Med.* 1987, **5**(3), 53-56 (Japan.) (*Chem. Abstr.* **107**, 70101k).
31. Sun, S. et al *Zhongguo Linchuang Yaoli Zazhi* 1990, **6**(4), 225-230.
32. Ali, S. L. *Anal. Profiles Drug Subst.* 1984, **13**, 597-653.
33. *Gov. Rep. Announce. Index (U. S.)* 1989, **89**(24), 1-231, Abstr. No. 965220, Natl. Tech. Inf. Ser. PB89-233589, Springfield, VA, USA

T63 tetradifon



$C_{12}H_6Cl_4O_2S$

Mol. Wt. 356.06

CAS Registry No. 116-29-0

Synonyms 1,2,4-trichloro-5-[(4-chlorophenyl)sulfonyl]benzene; *p*-chlorophenyl 2,4,5-trichlorophenyl sulfone; 2,4,5,4'-tetrachlorodiphenyl sulfone; Acaricide; Acaroil TD; Mitifon; Pinofon; Remanex; Roztoczol; Tedion

EINECS No. 204-134-2

RTECS No. WR 5850000

Uses Acaricide. Ovicide.

Physical properties

M. Pt. 148-149°C (pure); $\geq 144^\circ\text{C}$ (technical) **Specific gravity** 1.515 at 20°C **Partition coefficient** $\log P_{ow}$ 4.61 (1)

Volatility v.p. 7.5×10^{-3} mmHg at 20°C

Solubility Water: 80 $\mu\text{g l}^{-1}$ at 20°C. Organic solvents: acetone, benzene, chloroform, cyclohexanone, 1,4-dioxane, kerosene, methanol, toluene, xylene

Ecotoxicity

Fish toxicity

LC₅₀ (3 hr) carp $>10 \text{ mg l}^{-1}$ (2).

Guppies exposed to 1 mg l⁻¹ for 5 hr showed signs of poisoning; recovery was complete when transferred to clean water (3).

LC₅₀ (96 hr) bluegill sunfish, rainbow trout, channel catfish 880, 1200, 2100 $\mu\text{g l}^{-1}$, respectively (technical grade) 18-24°C (4).

Invertebrate toxicity

LC₅₀ (24, 48, 96 hr) scud 370, 140, 110 $\mu\text{g l}^{-1}$, respectively, (technical formulation) pH 7.1 and 23.8°C (5).

EC₅₀ (48 hr) *Daphnia magna* 0.2 or 2.0 mg l⁻¹. No toxic effects observed (1).

No inhibition of growth in *Chlorella pyrenoidosa* (96 hr) 2 mg l⁻¹ exposure (1).

EC₅₀ (short-term exposure) for toxic anorexia *Daphnia magna* filtration and ingestion rates towards the unicellular alga *Nannochloris oculata*, 0.02 and 0.24 mg l⁻¹, respectively (6).

LD₅₀ oral bee $>160 \mu\text{g}$ active ingredient bee⁻¹ (7).

Bioaccumulation

Not detected in the tissues of 750 freshwater fish samples (detection level 0.05 mg kg⁻¹) (8).

Environmental fate

Degradation studies

On an irrigated field sprayed at a rate of 10 kg ha⁻¹, only small amounts were found at deep levels. Transport through the soil was not affected by the amounts of water applied. Tetradifon persisted throughout the irrigation season (9).

A sandy loam soil was incubated aerobically for 106 wk. 70% of tetradifon was recovered unchanged and 20% as metabolites (1).

In a water/sandy loam hydrosol $t_{1/2}$ 36 wk, with almost all tetradifon retained in the soil phase. Under more aerobic conditions degradation was rapid with 69% degradation after 32 wk (1).

Adsorption and retention

Movement of tetradifon and partially degraded compound was investigated. Neither compound leached into groundwater (1).

Mammalian & avian toxicity

Acute data

LC₅₀ (4 hr) rat >3 mg l⁻¹ air (10).
LD₅₀ oral rat >14.7 g kg⁻¹ (2).
LD₅₀ oral dog 2000 mg kg⁻¹ (11).
LD₅₀ dermal rabbit 10 g kg⁻¹ (2).
LD₅₀ intraperitoneal mouse 75 mg kg⁻¹ (12).

Sub-acute and sub-chronic data

Oral rat (2 month) 500, 1000 mg kg⁻¹ in feed, no adverse effects observed (2).
Oral rat (90 day) 0, 50, 200, 1000, 3000 mg kg⁻¹ (diet), no growth retardation observed; 200 mg kg⁻¹ caused histological changes to the thyroid; liver weight increased at 1000 mg kg⁻¹ (13).
LC₅₀ (8 day) oral bobwhite quail, Japanese quail, pheasant, mallard duck >5000 mg kg⁻¹ (diet) (2).

Carcinogenicity and chronic effects

Oral rat (2 yr) 300 mg kg⁻¹ in feed, no adverse effects observed (2).
Oral rat (2 yr) 0, 30, 100, 300, 1200, 5000 or 20,000 mg kg⁻¹ (diet). At concentrations ≥1200 mg kg⁻¹ degenerative changes developed in liver and kidney (1).
Gavage mice (18 month) 100 mg kg⁻¹ did not induce tumours (14).

Metabolism and toxicokinetics

Oral rat, following single unspecified dose, 70% was excreted via the bile in the faeces within 48 hr (2).
Oral rat (10 day) 10 mg day⁻¹ (diet), elimination occurred via faeces and urine, although levels were detected in the fat, gastro-intestinal tissue, liver and muscle (15).
Oral rats single dose 1 mg, total recovery of the dose was 75% after 96 hr, predominantly in the faeces, 2-4% in urine, and 11% in carcass. Residues were detected in fatty tissue, plasma and lung. Unchanged compound was not detected in any of the urine or bile samples (1).

Irritancy

0.5 g technical grade compound was applied to rabbit skin. No irritation was observed. The formulation Tediion EC-8 caused mild irritation to rabbit skin when applied at a concentration of 0.5 ml (this concentrate contains 80 g l⁻¹ in xylene). 100 mg (technical grade) instilled into rabbit eye caused mild irritation (1).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA102 with metabolic activation negative (16).
In vivo mouse bone marrow 24, 48, 72 hr test samples for micronuclei negative (16).
In vitro human lymphocytes sister chromatid exchanges negative (17).

Other effects

Any other adverse effects

Intraperitoneal ♂ rats 40 mg kg⁻¹ caused slightly elevated plasma cholesterol levels 7 days after administration. Threshold levels were achieved 21 days after treatment (18).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (19).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (20).
 WHO Toxicity Class Table 5 (21).
 EPA Toxicity Class III (formulation) (10).
 The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th Amendments) (22).

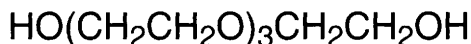
Other comments

Properties and hazards reviewed (23).
 Utilisation of by-products and wastes from manufacture discussed (24).
 One of a number of chemicals discharged into the Rhine, surrounding soil and air following an explosion at a Sandoz facility in 1986. No residual effects to water, sediment or biota were attributed to tetradifon (25).
 Identity and toxicity of chemicals discharged into Rhine and safety precautions for future spills reviewed (26).

References

1. *Environmental Health Criteria No. 67: Tetradifon 1986*, WHO, Geneva, Switzerland.
2. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
3. Adlung, K. G. *Naturwissenschaften* 1957, **44**, 471-472.
4. Johnson, W. W. et al *Handbook of Acute Toxicity to Fish and Aquatic Invertebrates* 1980, 1-75, US Fish & Wildlife Ser., No. 137, Washington, DC, USA.
5. Sanders, O. *Toxicity of Pesticides to the Crustacean, Gammarus lacustris* 1969, 1-18, US Dept. Fish and Wildlife Ser., Technical Paper No. 25, Washington, DC, USA.
6. Villarroel, M. J. et al *J. Environ. Sci. Health, Part B* 1998, **B33**(2), 151-160.
7. Oomen, P. A. *Meded. Fac. Landsbouwwet. Rijksuniv. Gent* 1986, **51**(3b), 1205-1213.
8. Chovelon, A. et al *Chemosphere* 1984, **13**(1), 19-32.
9. Yaron, B. et al *J. Environ. Qual.* 1974, **3**, 413-417.
10. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
11. *Spec. Publ. Entomol. Soc. Am.* 1978, **78**(1), 55.
12. Ishida, K. et al *Niigata Norin Kenkyu* 1969, **21**, 183-201.
13. Verschuuren, H. G. et al *Toxicologist* 1973, **1**, 113-123.
14. Innes, J. R. M. et al *J. Natl. Cancer Inst.* 1969, **42**, 1101-1104.
15. Halberstadt, J. *Meded. Landbouwhogeschool Gent* 1958, **23** 788-794.
16. Chruscielska, K. et al *Pestycydy (Warsaw)* 1991, **1**, 35-39 (Pol.) (*Chem. Abstr.* **115**, 177056s).
17. Sobti, R. C. et al *Arch. Toxicol.* 1983, **52**, 221-231.
18. Ishikawa, T. T. et al *Metabolism* 1978, **27**, 89-96.
19. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
20. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
21. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
22. *1967 Directive on Classification, Packaging and Labelling of Dangerous Substances* 67/548/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
23. *Dangerous Prop. Ind. Mater. Rep.* 1989, **9**(1), 44-50.
24. Skotnicki, E. *Przem. Chem.* 1988, **67**(4), 177-179 (Pol.) (*Chem. Abstr.* **109**, 233099y).
25. Capel, P. D. *Comm. Eur. Communities, [Rep.] EUR* 1988, 189-194, EUR 11350.
26. Binnemann, P. H. *GIT – Suppl.* 1988, **2**, 54-56, 58-60, 62-63 (Ger.) (*Chem. Abstr.* **109**, 98383u)

T64 tetraethylene glycol



C₈H₁₈O₅

Mol. Wt. 194.23

CAS Registry No. 112-60-7

Synonyms 2,2'-(oxybis(ethyleneoxy))diethanol; Hi-Dry; TEG

EINECS No. 203-989-9

RTECS No. XC 2100000

Physical properties

M. Pt. -6°C B. Pt. 314°C Flash point 176°C (open cup) Specific gravity 1.125 at 20°C with respect to water at 20°C Partition coefficient log P_{ow} -1.38/-2.18 (calc.) Volatility v.p. 0.001 mmHg at 20°C; v.den. 6.7
Solubility Water: miscible. Organic solvents: diethyl ether, ethanol

Ecotoxicity

Fish toxicity

Trout, bluegill sunfish, yellow perch and goldfish were exposed to 5 ppm for 24 hr; no toxic effects observed. Test conditions: pH 7.0; dissolved oxygen content 7.5 ppm; total hardness (soap method) 300 ppm; methyl orange alkalinity 310 ppm; free carbon dioxide 5 ppm; at 12.8°C (1).

Environmental fate

Degradation studies

BOD₁₋₁₀ feed 200-1000 mg l⁻¹ (20°C) acclimation 365+ days (2).

Abiotic removal

Activated carbon: adsorbability 0.116 g g⁻¹ carbon; 58.1% reduction influent 1000 mg l⁻¹; effluent 418 mg l⁻¹ (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 33 g kg⁻¹ (4).

Teratogenicity and reproductive effects

Intragastric rats (unspecified dose) administered on day 19 of gestation or inhalation rats 4 hr day⁻¹ (unspecified dose) throughout pregnancy caused embryonic and teratogenic effects. No-effect dose was 0.002% of LD₅₀ (5). Intragastric ♂ rats (2-6 month) 0.0002-0.02 LD₅₀ caused decreases in cytochrome oxidase activity in the testis and alkaline phosphatase activity in the epididymis. Testis damage and increased incidence of abnormal sperm were observed. Malformation of central nervous system and skeleton were observed in the offspring of the treated ♂ (6).

Irritancy

Dermal rabbit (unspecified duration) 550 mg (open) caused mild irritation (7).

Other effects

Any other adverse effects

Administration to rats (route and dose unspecified) produced changes in the function and morphology of liver, kidneys and central nervous system. The toxic effects were dose dependent. Adverse effects on gonads, blood indices and embryonic development were also noted (8).

Legislation

The recommended maximum permissible concentration in water treatment uses is 2 mg l⁻¹ (8).

Other comments

Reviews on human health effects and experimental toxicology listed (9).

References

1. *The Toxicity of 3400 Chemicals to Fish* 1987, EPA560/6-87-002, PB87-200-275, Washington, DC, USA.
2. Ludzak, F. J. et al *JWPCF, J. Water Pollut. Control Fed.* 1960, **32**, 1173.
3. Guishi, D. M. et al *JWPCF, J. Water Pollut. Control Fed.* 1974, **46**(5), 947-965.
4. *Material. Safety Data Sheet* 1978, Dow Chemical Corp., New York, NY, USA.
5. Barilyak, I. R. *Fiziol. Akt. Veshchestva* 1989, **21**, 30-33 (Russ.) (*Chem. Abstr.* **113**, 93155u).
6. Byshovets, T. F. et al *Gig. Sanit.* 1987, **9**, 84-85 (Russ.) (*Chem. Abstr.* **107**, 192758a).
7. *Union Carbide Data Sheet* 1969, Union Carbide Corporation, New York, NY, USA.
8. Tolstopystova, G. V. et al *Gig. Sanit.* 1987, **12**, 77-78 (Russ.) (*Chem. Abstr.* **108**, 128330y).
9. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T65 tetraethylenepentamine



$\text{C}_8\text{H}_{23}\text{N}_5$

Mol. Wt. 189.30

CAS Registry No. 112-57-2

Synonyms N-(2-aminoethyl)-N'-[2-[(2-aminoethyl)amino]ethyl]-1,2-ethanediamine; DEH 26; 1,4,7,10,13-pentaazatridecane; 3,6,9-triazaundecamethylenediamine; 3,6,9-triazaundecane-1,11-diamine

EINECS No. 203-986-2

RTECS No. KH 8585000

Uses Chemical intermediate. Coagulation aid for synthetic rubber latices. Corrosion inhibition. Catalyst. Solvent.

Physical properties

M. Pt. -40°C **B. Pt.** 340°C **Flash point** 185°C **Specific gravity** 0.9980 at 20°C with respect to water at 20°C

Partition coefficient $\log P_{\text{ow}}$ -1.503 (1) **Volatility** v.p. 8×10^{-7} mmHg at 25°C; v.den. 6.53

Solubility Water: miscible

Occupational exposure

UN No. 2320 **HAZCHEM Code** 2X **Conveyance classification** corrosive substance

Supply classification corrosive, dangerous for the environment

Risk phrases Harmful in contact with skin and if swallowed – Causes burns – May cause sensitisation by skin contact – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R21/22, R34, R43, R51/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S26, S36/37/39, S45, S61)

Ecotoxicity

Bioaccumulation

Estimated bioconcentration factor 4.2 indicates that environmental accumulation is unlikely (2).

Environmental fate

Abiotic removal

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated $t_{1/2}$ 1.2 hr (3).

Adsorption and retention

Estimated K_{oc} of 3.6 indicates that adsorption to soil and sediments will not occur (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 2100-3990 mg kg⁻¹ (4,5).

LD₅₀ dermal rabbit 660 mg kg⁻¹ (6).

LD₅₀ intravenous mouse 320 mg kg⁻¹ (7).

LD₅₀ intraperitoneal rat 205 mg kg⁻¹ (8).

Carcinogenicity and chronic effects

Dermal ♂ mouse 25 µl 3 × wk⁻¹ for life. No skin tumours were reported. Hyperkeratosis occurred in 20/50, and epidermal necrosis occurred in 13/50 treated mice (9).

Irritancy

Dermal rabbit 500 mg caused severe irritation and 5 mg instilled into rabbit eye caused moderate irritation (exposure unspecified) (10).

Genotoxicity

Salmonella typhimurium TA100 with and without metabolic activation positive (11).

Drosophila melanogaster sex-linked recessive lethal assay negative (12).

Other effects

Any other adverse effects

Exhibited potent inactivation of copper-superoxide dismutase activity in the rat liver and caused hepatic necrosis (13).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (14).

Other comments

pK_a values of 2.98-9.68 indicate that the compound will exist primarily as the cation in environmental conditions (15).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (16).

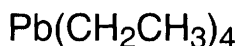
Autoignition temperature 300°C.

References

1. *Graphical Exposure Modelling System* 1987, US EPA, Office of Toxic Substances, Washington, DC, USA.
2. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
3. Atkinson, R. *Environ. Toxicol. Chem.* 1988, 7, 435-442.
4. Gosselin, R. E. et al *Clinical Toxicology of Commercial Products* 5th ed., 1984, II, 207, Williams & Wilkins, Baltimore, MD, USA.
5. *Kirk-Othmer Encyclopedia of Chemical Toxicology* 3rd ed., 1979, 7, 591, John Wiley and Sons, NY, USA.
6. *J. Ind. Hyg. Toxicol.* 1949, 31, 60.
7. *Report NX 03522M* US Army Armament Res. Dev. Command, Chemical Systems Laboratory, Aberdeen Proving Ground, MD 21010, USA.
8. *Inorg. Chim. Acta* 1984, 91, L51.
9. De Pass, L. R. et al *Fundam. Appl. Toxicol.* 1987, 9(4), 807-811.

10. *Union Carbide Data Sheet* 21 March 1973.
11. Mortelmans, K. et al *Environ. Mutagen.* 1986, **8**(Suppl. 7), 1-119.
12. Zimmering, S. et al *Environ. Mol. Mutagen.* 1989, **14**(4), 245-251.
13. Ishiyama, H. et al *Pharmacol. Toxicol. (Copenhagen)* 1991, **69**(3), 215-217.
14. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
15. Perrin, D. D. *Dissociation Constant for Organic Bases in Aqueous Solution* 1965, IUPAC Chemical Data Series No. 4014, Butterworth, London, UK.
16. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T66 tetraethyllead



$\text{C}_8\text{H}_{20}\text{Pb}$

Mol. Wt. 323.45

CAS Registry No. 78-00-2

Synonyms lead tetraethyl; TEL; tetraethylplumbane

EINECS No. 201-075-4

RTECS No. TP 4550000

Uses As a gasoline additive to prevent 'knocking' in motors.

Physical properties

M. Pt. -130°C B. Pt. 227.7°C (decomp.) Flash point 93.3°C Specific gravity 1.653 at 20°C

Volatility v.p. 0.2 mmHg at 20°C ; v.den. 8.6

Solubility Water: 0.29 mg l^{-1} at 25°C . Organic solvents: benzene, diethyl ether, ethanol, light petroleum

Occupational exposure

DE-MAK 0.05 mg m^{-3} (as Pb)

FR-VME 0.1 mg m^{-3} (as Pb)

JP-OEL 0.075 mg m^{-3} (as Pb)

SE-LEVL 0.05 mg m^{-3} (as Pb)

SE-STEEL 0.2 mg m^{-3} (as Pb)

UK-LTEL 0.10 mg m^{-3} (as Pb)

US-TWA 0.1 mg m^{-3} (as Pb)

UN No. 1649 HAZCHEM Code 2WE Conveyance classification toxic substance

Supply classification very toxic

Supply classification dangerous for the environment

Risk phrases May cause harm to the unborn child – Possible risk of impaired fertility – Very toxic by inhalation, in contact with skin and if swallowed – Danger of cumulative effects – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R61, R62, R26/27/28, R33, R50/53)

Safety phrases Avoid exposure – obtain special instruction before use – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S53, S45, S60, S61)

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) bass 0.065 mg l^{-1} static bioassay at 20°C (1).

LC₅₀ (24, 48, 96 hr) bluegill sunfish 2.0-0.02 mg l^{-1} static bioassay at pH 6.9-7.5, 20°C , alkalinity 33-81 mg l^{-1} (CaCO_3), hardness 84-163 mg l^{-1} (CaCO_3) (2).

LC₅₀ (96 hr) plaice 0.23 mg l⁻¹ flow through bioassay at 15°C and 34.9 mg l⁻¹ (CaCO₃) salinity (3).
LC₅₀ (48 hr) stickleback, coho salmon 14 µg l⁻¹ for effluent discharges from tetraethyllead production plants. No attempt was made to assess the indirect hazard caused to birds by food organisms concentrating the lead (4).

Invertebrate toxicity

EC₅₀ (4 hr) *Ankistrodesmus falcatus* <0.3 mg l⁻¹ (5).
Poteroiuchromonas malhamensis (3 day) 100 mg l⁻¹ cultured in dark suffered no toxic effects, in light all cells were killed at 80 mg l⁻¹. In light, <80 mg l⁻¹ caused dose-related effects on growth, mitosis and cytokinesis. Conversion into a highly toxic derivative (triethyllead) took place within 3-6 hr, maximum concentration 24-32 hr (6).
Compounds used to alleviate lead poisoning in humans (including EDTA salts, dimercaprol) increased the effects of triethyllead on *Poteroiuchromonas malhamensis* (7).
LC₅₀ (96 hr) mussel, brown shrimp 0.1 mg l⁻¹ and 0.02 mg l⁻¹ (flowthrough), at 15°C and 34.9‰ salinity (3).
It is non-toxic to freshwater and marine algae (duration and concentration unspecified); the trialkyllead degradation product is responsible for the apparent toxicity of tetraethyllead (8).
Scrobicularia plana did not suffer any siphonal contraction when pure tetraethyllead was applied to the preparation. It has a low toxicity or is non-toxic in pure form (9).

Bioaccumulation

In Canada, northern pike and redhorse sucker living in rivers near alkyllead production plants contained 0.17 and 5.04 µg g⁻¹, respectively (10).
Caged clams concentrated tetraethyllead in the muscle and visceral tissues (10).
Accumulation (96 hr) in shrimp at 0.02 mg l⁻¹ gave a concentration factor of 650 (5).
Accumulation (96 hr) *Mytilus edulis* at 10 mg l⁻¹ gave a mean concentration factor of 120 for digestive gland, foot, gill and gonad (11).
Accumulation (96 hr) plaice at 0.23 mg l⁻¹ gave a concentration factor of 130 (11).

Environmental fate

Degradation studies

BOD using mixed coastal marine bacteria, concentrations <0.16 mg l⁻¹ O₂ had no significant effect on lag phase.
EC₅₀ (48 hr) 0.2 mg l⁻¹ (1).
EC₅₀ (48 hr) *Dunaliella tertiolecta* 0.15 mg l⁻¹ (1).
Tetraalkyllead compounds are the predominant alkyllead compounds in the atmosphere. They are removed from the air in rainwater and transferred to surface and highway drainage water, where sequential breakdown of tetraalkyllead to tri- and dialkyllead compounds occurs (12).

Mammalian & avian toxicity

Acute data

LD₅₀ oral Japanese quail 24.6 mg kg⁻¹ (13).
LD₅₀ oral mallard duck 107 mg kg⁻¹ (13).
LD₅₀ oral rat 12.3 mg kg⁻¹ (14).
LD_{Lo} oral rabbit 30 mg kg⁻¹ (15).
LD_{Lo} dermal dog, guinea pig 547, 995 mg kg⁻¹, respectively (15).
LD₅₀ intravenous rat, rabbit 15, 22 mg kg⁻¹, respectively (16,17).
LD_{Lo} subcutaneous rabbit 32 mg kg⁻¹ (17).

Sub-acute and sub-chronic data

Oral starling (11 day) 0, 200, 2000 µg l⁻¹. All birds receiving low doses survived treatment. Lead accumulated in the brain, kidney and liver (18).
Mallard ducks, Japanese quail (6 day) 6 mg kg⁻¹ body weight, no effect on eggshell thickness (19).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (20).

Teratogenicity and reproductive effects

Oral Simonsen Sprague-Dawley rats 7.5, 15 or 30 mg kg⁻¹ body weight on 3 consecutive days (9, 10, 11 or 12, 13, 14) of organogenesis. Doses up to those lethal to some mother animals were essentially non-teratogenic to offspring (21).

Transplacental effects of tetraethyllead on tissue plasminogen activator activity, plasminogen activator inhibition and plasma inhibition were studied in rats. Changes in these processes were observed in lungs, liver, heart, brain and kidneys. Foetal tissue plasminogen activator activity, plasminogen activator inhibition and plasma inhibition can be affected transplacentally by tetraethyllead (22).

Metabolism and toxicokinetics

Tissue distribution studies of lead in rats and dogs exposed by inhalation revealed lead levels of 7-100 mg kg⁻¹ tissue in lung, brain, liver, kidney, spleen and heart (23).

Oral, intravenous (duration unspecified) or inhalation (5 hr) rabbits at 3 mg, 12 mg or 200 µg m⁻³ air, respectively. Correlation was observed between diethyllead excretion in urine and the dose and method of administration (24).

Other effects

Other adverse effects (human)

Seven occupationally exposed workers had altered plasma renin activity. The changes are discussed with regard to neurogenic, hormonal, humoral and electrolyte factors influencing the release of renin (25).

All malignant neoplasms detected in the active and pensioned employees of the Du Pont tetraethyllead production plant during 1956-1987 were studied. The 735 cases were compared with matched controls and their exposure to chemicals in the tetraethyllead manufacturing process was estimated. There was a strong association between exposure and both rectal and sigmoid colon cancers. An exposure-response relationship was observed, with a four-fold elevation in the odds ratio at high cumulative exposure levels. The findings were consistent with the colorectal cancer experience at the plant, but the causal role was not established (26).

Any other adverse effects

In rats with cerebral oedema induced by tetraethyllead, brain mitochondrial monophosphoinositides, sphingomyelins and phosphatidylserines, phosphatidylethanolamines and cardiolipins increased. Decrease in monophosphoinositides, phosphatidylcholines and phosphatidylethanolamines in brain microsomes. Increases in lysophosphatidylcholines and sphingomyelins were observed. Increased lipid peroxidation also accompanied cerebral oedema (27).

In 1979, 2400 birds were found dead or dying in the Mersey estuary, UK, the majority being waders. Smaller numbers of dead birds were found in 1980 and 1981. A plant manufacturing petrol additives was in the vicinity. Affected birds contained elevated lead levels mostly as alkyllead (28).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (29).

Other comments

Generally tetraalkyllead compounds are of higher toxicity to microorganisms than inorganic lead compounds. Organolead compounds are generally 10-100 × more toxic to aquatic organisms than inorganic leads.

Tetraalkyllead becomes toxic by conversion into trialkyllead (30).

Acute or chronic poisoning may occur if inhaled or absorbed through skin (31).

Dilute solution in water decomposes to give triethyl salt, then diethyl salt and finally inorganic lead (32).

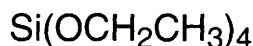
Lead from tetraethyllead in soil and vegetation decreases exponentially with the distance from the road. Levels in plants and animals increase in areas close to roads; the levels are positively correlated with traffic volume and proximity of roads (30).

Hazardous properties reviewed (33).

References

1. Marchetti, R. *Mar. Pollut. Bull.* 1978, **9**, 206-207.
2. Turnbull, H. et al *Ind. Eng. Chem.* 1954, **46**, 324-333.
3. Maddock, B. G. et al *Lead in the Marine Environment* 1980, 233-261, Pergamon Press, Oxford, UK.
4. Gill, J. M. et al *J. Water Pollut. Control Fed.* 1960, **32**, 858-867.
5. Silverberg, B. A. et al *Arch. Environ. Contam. Toxicol.* 1977, **5**, 305-313.
6. Roderer, G. *Environ. Res.* 1980, **23**, 371-384.
7. Roderer, G. *Chem.-Biol. Interact.* 1983, **48**, 247-254.
8. Jarvie, A. W. P. *Appl. Organomet. Chem.* 1987, **1**(1), 29-38.
9. Marshall, S. J. et al *Appl. Organomet. Chem.* 1988, **2**(2), 143-149.
10. Chau, Y. K. et al *Chem. Environ. Proc. Int. Conf.* 1986, 77-82.
11. Grove, J. R. *Investigation into the formation and behaviour of aqueous solutions of lead alkyls*, The Associated Octel Co. Ltd., Ellesmere Port, UK.
12. Radojevic, M. *Heavy Met. Environ., Int. Conf. 5th* 1985, **1**, 82-84.
13. Hudson, R. H. et al *Handbook of toxicity of pesticides to wildlife* 2nd ed., 1984, US Dept. Int., Fish & Wildlife Ser., Report No. 153, Washington, DC, USA.
14. Schroeder et al *Experientia* 1972, **28**, 923.
15. *Jpn. J. Ind. Health* 1973, **15**, 3.
16. *Ind. Med.* 1963, **54**, 486.
17. *Environ. Qual. Saf., Suppl.* 1975, **1**, 1.
18. Osborn, D. et al *Environ. Pollut.* 1983, **31**, 261-275.
19. Haegele, M. A. et al *Bull. Environ. Contam. Toxicol.* 1974, **11**, 98-102.
20. *IARC Monograph* 1987, **Suppl. 7**, 230-232.
21. McClain, R. M. et al *Toxicol. Appl. Pharmacol.* 1972, **21**, 265-274.
22. Smokovitis, A. et al *Biol. Neonate* 1990, **58**(1), 41-49.
23. Davies, B. E. et al *Arch. Environ. Health* 1963, **6**, 473-479.
24. Kozarzewska, Z. et al *Br. J. Ind. Med.* 1987, **44**(6), 417-421.
25. Carmignani, M. et al *Acta Med. Rom.* 1988, **26**(3), 277-286.
26. Fayerweather, W. E. et al *Am. J. Ind. Med.* 1997, **31**(1), 28-35.
27. Pogosyan, A. Y. et al *Biol. Zh. Arm.* 1989, **42**(1), 37-41 (Russ.).
28. Head, P. C. et al *The Mersey Estuary bird mortality Autumn-Winter 1979 – preliminary report* 1980, Directorate of Scientific Services, Report No. DSS-EST-80-1, Warrington, UK.
29. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
30. *IPCS Environmental Health Criteria 85: Lead – Environmental Aspects* 1989, WHO, Geneva, Switzerland.
31. Browning, E. *Toxicity of Industrial Metals* 2nd ed., 1969, 192-199, Appleton-Century-Crofts, London, UK.
32. Harrison, G. F. *The Cavtat Incident* 1977, presented at the International Experts Discussion Meeting on Lead - Occurrence, Fate and Pollution in the Marine Environment, Rovinj, Croatia.
33. *Dangerous Prop. Ind. Mater. Rep.* 1989, **9**(4), 77-87

T67 tetraethyl orthosilicate



$\text{C}_8\text{H}_{20}\text{O}_4\text{Si}$

Mol. Wt. 208.33

CAS Registry No. 78-10-4

Synonyms ethyl silicate; tetraethyl silicate; tetraethoxysilane; Dynasil A; ES 28; ES 100; silicon ethoxide; silicon tetraethoxide; Silikan L

EINECS No. 201-083-8

RTECS No. VV 9450000

Uses Cross-linking catalyst. Manufacture of surface coatings. Used for hardening stone to arrest decay and disintegration.

Physical properties

M. Pt. -77°C **B. Pt.** 168°C **Flash point** 43°C (open cup) (99.9% purity) **Specific gravity** 0.933 at 20°C with respect to water at 4°C **Volatility** v.p. 1.0 mmHg at 20°C; v.den. 7.22
Solubility Organic solvents: ethanol

Occupational exposure

DE-MAK 10 ppm (86 mg m⁻³)

FR-VME 10 ppm (85 mg m⁻³)

JP-OEL 10 ppm (85 mg m⁻³)

UK-LTEL 10 ppm (87 mg m⁻³)

UK-STEL 30 ppm (260 mg m⁻³)

US-TWA 10 ppm (85 mg m⁻³)

UN No. 1292 **HAZCHEM Code** 3Y **Conveyance classification** flammable liquid

Supply classification harmful

Risk phrases Flammable – Harmful by inhalation – Irritating to eyes and respiratory system (R10, R20, R36/37)

Safety phrases Keep out of reach of children (if sold to general public) (S2)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 6300 mg kg⁻¹ (1).

LC_{Lo} (4 hr) inhalation rat 1000 ppm (1).

LD₅₀ dermal rabbit 5900 mg kg⁻¹ (2).

LD_{Lo} intravenous rabbit 200 mg kg⁻¹ (3).

Sub-acute and sub-chronic data

Inhalation mouse, 1000 ppm for 1, 2, 4 or 8 hr, or 200 ppm for 6 hr day⁻¹, 5 days wk⁻¹ for 2 or 4 wk. Behaviour was affected in all mice exposed to 1000 ppm. Some fatalities also occurred in these groups. Histopathological examination revealed scarring of the renal cortex, acute tubular necrosis and atrophy of the spleen. There were no significant abnormalities in clinical chemistry values (4).

Irritancy

Dermal rabbit (24 hr) 500 mg caused moderate irritation, 100 mg instilled into rabbit eye (exposure not specified) caused mild irritation (2).

Other effects

Other adverse effects (human)

Narcotic at high concentration (5).

Any other adverse effects

Intraperitoneal mouse, 10-2000 mg kg⁻¹ caused death in 20/26 mice administered ≥830 mg kg⁻¹. The body weight in these groups decreased. Renal damage, pleural effusion, splenic discoloration and a decrease in splenic volume were observed in dead animals. The deposition of basophilic granules in the bronchi was observed in 70% of mice given ≥1670 mg kg⁻¹ (6).

Other comments

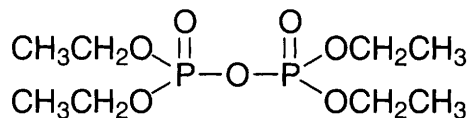
Reviews on human health effects, experimental toxicology, physico-chemical properties listed (7).

References

1. *J. Ind. Hyg. Toxicol.* 1949, **31**, 40.
2. *Union Carbide Data Sheet* 23 July 1970.
3. *Ind. Med.* 1939, **6**, 660.
4. Setoguchi, T. et al *Nippon Sanso Giho* 1990, (9), 68-72. (Japan.) (*Chem. Abstr.* **114**, 158775p).
5. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.

6. Nakashima, H. et al *Sangyo Igaku* 1991, 33(4), 256-257 (Japan.) (*Chem. Abstr.* 115, 200534g).
7. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T68 tetraethyl pyrophosphate



C₈H₂₀O₇P₂

Mol. Wt. 290.19

CAS Registry No. 107-49-3

Synonyms diphosphoric acid, tetraethyl ester; pyrophosphoric acid, tetraethyl ester; bis-O,O-diethylphosphoric anhydride; TEPP; Bladan; Killex; Pyroduct

EINECS No. 203-495-3

RTECS No. TX 6825000

Uses Superseded insecticide and rodenticide.

Physical properties

M. Pt. 170-213°C (decomp.) **B. Pt.** 124°C at 1 mmHg **Specific gravity** 1.185 at 20°C with respect to water at 4°C **Volatility** v.p. 155×10^{-6} mmHg at 20°C

Solubility Water: miscible, but quickly hydrolysed. Organic solvents: miscible with acetone, benzene, carbon tetrachloride, chloroform, ethanol, ethylene glycol, glycerol, methanol, propylene glycol, toluene, xylene

Occupational exposure

DE-MAK 0.005 ppm (0.060 mg m⁻³)

FR-VME 0.004 ppm (0.05 mg m⁻³)

UK-LTEL 0.004 ppm (0.05 mg m⁻³)

UK-STEL 0.01 ppm (0.12 mg m⁻³)

US-TWA 0.05 mg m⁻³

Supply classification very toxic, dangerous for the environment

Risk phrases Very toxic in contact with skin and if swallowed – Very toxic to aquatic organisms (R27/28, R50)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Wear suitable protective clothing, gloves and eye/face protection – In case of insufficient ventilation, wear suitable respiratory equipment – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S36/37/39, S38, S45, S61)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow, bluegill sunfish 1.1-1.9 mg l⁻¹ (1).

Sockeye salmon, steelhead trout and threespine stickleback exposed to 10 mg l⁻¹ (40% active ingredient) in a 24 hr bioassay showed no ill-effects. Test conditions: artesian well water, total hardness 67-120 mg l⁻¹; methyl orange alkalinity 151-183 mg l⁻¹; total dissolved solids 160-175 mg l⁻¹; and pH 7.1 (2).

Trout, bluegill sunfish, and yellow perch exposed to 5 ppm for 24 hr showed signs of sickness within 22, 6 and 4 hr, respectively. Goldfish exposed to 5 ppm for 24 hr showed no ill-effects. Test conditions: pH 7; dissolved oxygen content 7.5 ppm; total hardness (soap method) 300 ppm; methyl orange alkalinity 310 ppm; free carbon dioxide 5 ppm; and 12.8°C (3).

Invertebrate toxicity

LOEC (10 day) *Chlorella* sp., *Phaeodactylum tricornutum*, *Monochrysis lutheri* 10 mg l⁻¹ (4).

LC₅₀ (96 hr) *Gammarus lacustris* 0.039 mg l⁻¹ (5).

LC₅₀ (48 hr) *Grassostrea virginica* 1 × 10⁴ ppb (laboratory, static bioassay) (4).

Environmental fate

Abiotic removal

Hydrolysed in water, t_{1/2} 7 hr at 25°C (50% v/v mixture) (6).

Mammalian & avian toxicity

Acute data

LD₅₀ oral ♂ rat 1.1 mg kg⁻¹ (7).

LD₅₀ oral mouse 7 mg kg⁻¹ (8).

LD₅₀ dermal rat 2.4 mg kg⁻¹ (8).

Other effects

Any other adverse effects

Cholinesterase inhibitor (species unspecified) (9).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (10).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (11).

Other comments

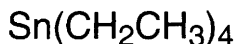
Reviews on human health effects, experimental toxicology, ecotoxicology and physico-chemical properties listed (12).

Hygroscopic.

References

1. Pickering, Q. H. et al *Trans. Am. Fish. Soc.* 1962, **91**(2), 175-184.
2. *Lethal Effects of 2014 Chemicals Upon Sockeye Salmon, Steelhead Trout and Threespine Stickleback* 1989, US EPA560/6-89-001, PB89-156715, Washington, DC, USA.
3. *The Toxicity of 3400 Chemicals to Fish* 1987, US EPA560/6-87-002, PB87-200-275, Washington, DC, USA.
4. Davis, H. C. et al *Fish. Bull.* 1969, **67**(2), 383-404.
5. Sanders, H. O. *Toxicity of Pesticides to the Crustacean Gammarus lacustris* 1969, Bureau of Sport, Fisheries and Wildlife, Technical Paper 25, Washington, DC, USA.
6. Verschuere, K. *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, Van Nostrand Reinhold, New York, NY, USA.
7. Gaines, T. B. *Toxicol. Appl. Pharmacol.* 1969, **14**, 515.
8. *Registry of Toxic Effects of Chemical Substances* 1984, NIOSH No. 83-107-4.
9. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
10. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
11. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
12. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T69 tetraethyltin



$\text{C}_8\text{H}_{20}\text{Sn}$

Mol. Wt. 234.96

CAS Registry No. 597-64-8

Synonyms tetraethylstannane

EINECS No. 209-906-2

RTECS No. WH 8625000

Uses Intermediate used in the preparation of other organotin compounds.

Physical properties

M. Pt. -112°C B. Pt. 181°C Flash point 53°C Specific gravity 1.187 at 23°C

Occupational exposure

DE-MAK 0.1 mg m^{-3} (as Sn) (total dust)

SE-LEVL 0.1 mg m^{-3} (as Sn)

SE-STEEL 0.2 mg m^{-3} (as Sn)

UK-LTEL 0.1 mg m^{-3} (as Sn)

UK-STEEL 0.2 mg m^{-3} (as Sn)

US-TWA 0.1 mg m^{-3} (as Sn)

US-STEEL 0.2 mg m^{-3} (as Sn)

UN No. 2810 HAZCHEM Code 2X (solid) Conveyance classification toxic substance

Ecotoxicity

Invertebrate toxicity

EC_{50} *Skeletonema costatum* 142-148 $\mu\text{g l}^{-1}$; *Thalassiosira pseudonana* 116-121 $\mu\text{g l}^{-1}$ (calculated by graphical interpolation, moving average, probit methods) (1).

Environmental fate

Abiotic removal

May absorb UV light $>290 \text{ nm}$ and may be susceptible to direct photolysis based on the absorption behaviour of tri-, di- and monobutyl compounds (2).

Mammalian & avian toxicity

Acute data

LD_{50} oral mouse, guinea pig 40, 37 mg kg^{-1} , respectively (3,4).

LD_{50} oral rabbit, rat 7, 15 mg kg^{-1} , respectively (3,4).

LD_{Lo} intravenous rat 25 mg kg^{-1} (5).

Metabolism and toxicokinetics

Intravenous rats, rabbits (dose and duration unspecified), dealkylation and dearylation occurred in the liver. The triethyltin metabolite was detected in the tissues (6,7).

Other effects

Other adverse effects (human)

In 1954 a serious incident of organotin poisoning occurred with a proprietary preparation of a drug used in the treatment of furunculosis, osteomyelitis, anthrax and acne. The drug was responsible for 100 deaths and 210 intoxications. The main ingredients were diethyltin dioxide ($15 \text{ mg capsule}^{-1}$) and linoleic acid ($100 \text{ mg capsule}^{-1}$). It was suggested that ethyltin triiodide, triethyltin iodide or tetraethyltin could have been present as impurities or metabolites. Main symptoms were headache, nausea, vomiting, visual disturbances, congestion, papilloedema and papillary stasis. Frequently occurring symptoms were urinary incontinence, vertigo, loss of weight and abdominal pains. Death occurred during coma or from respiratory or cardiac failure or convulsions (8-14).

Any other adverse effects

Intraperitoneal rats (dose and duration unspecified) decreased central dopamine and brain serotonin levels. The behavioural and autonomic effects suggest a central sympatholytic and antipsychotic type of sedation and rigidity (15).

In experimental animals, it can cause muscular weakness, paralysis, respiratory failure, tremors and hyperexcitability (16).

Intravenous dogs 25 mg kg⁻¹ produced a slight increase in the respiratory rate and vasodilation as immediate effects, but after 90-120 min, prostration with muscular weakness was noted (17).

Other comments

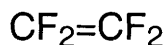
Impurity in triphenyltin acetate.

Tin and organotin compounds comprehensively reviewed (16).

References

1. Walsh, G. E. et al *Environ. Toxicol. Chem.* 1987, **6**, 767-770.
2. Maguire, R. J. et al *J. Agric. Food Chem.* 1983, **31**, 1060-1065.
3. Skackova, I. N. *Gig. Sanit.* 1967, **4**, 11-17.
4. Mazaev, V. T. et al *J. Hyg. Epidem. Microbiol. Immunol.* 1971, **15**(1), 115-120.
5. *Br. J. Pharmacol. Chemother.* 1955, **10**, 16.
6. Cremer, J. E. *Biochem. J.* 1958, **68**, 685-692.
7. Bridges, J. W. et al *Biochem. J.* 1967, **105**, 1261-1266.
8. Alajouanine, T. et al *Rev. Neurol.* 1958, **98**, 85-96.
9. Barnes, J. M. et al *Pharmacol. Rev.* 1959, **11**, 211-213.
10. Rondepierre, J. et al *Rev. Neurol.* 1958, **98**, 135-140.
11. Lecoq, R. C. R. *Hebd. Acad. Sci. (Paris)* 1954, **239**, 678-680.
12. Druault-Toufesco, M. N. *Bull. Soc. Ophthalmol. Fr.* 1955, 54-58.
13. Cossa, P. et al *Rev. Neurol.* 1958, **98**, 97-108.
14. Fontan, M. M. *J. Med. Bordeaux* 1955, **132**, 399-405.
15. Chester, A. E. et al *Proc. Soc. Exp. Biol. Med.* 1988, **187**(1), 62-68.
16. *Environmental Health Criteria No. 15: Tin and Organotin Compounds* 1980, WHO, Geneva, Switzerland.
17. Stoner, H. B. et al *Br. J. Pharmacol.* 1955, **10**, 16-25

T70 tetrafluoroethylene



C₂F₄

Mol. Wt. 100.02

CAS Registry No. 116-14-3

Synonyms tetrafluoroethene; perfluoroethene; perfluoroethylene; 1,1,2,2-tetrafluoroethylene; TFE

EINECS No. 204-126-9

RTECS No. KX 4000000

Uses In the manufacture of high PTFE homopolymer. Copolymerised with hexafluoropropylene, ethylene, perfluorinated ethers, isobutylene and propylene.

Physical properties

M. Pt. -142.5°C **B. Pt.** -76°C **Specific gravity** 1.519 at -76.3°C **Volatility** v.den. 3.9

Occupational exposure

UN No. 1081 (inhibited) **Conveyance classification** flammable gas

Mammalian & avian toxicity

Acute data

LC₅₀ (4 hr) inhalation rats 40,000 ppm (1).

LC₅₀ (duration unspecified) inhalation mouse, guinea pig 143, 116 g m⁻³, respectively (2).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (3).

National Toxicology Program tested mice and rats via inhalation. Clear evidence of carcinogenicity in ♂ and ♀ rats and mice (4).

Other effects

Any other adverse effects

Inhalation rats (6 hr) 6000 ppm caused kidney damage (1).

Inhalation ♂ rats (30 min) 3500 ppm in air caused no gross pathology of any of the organs, but small amounts of fluoride ion were excreted in the urine over a 14 day period indicating the compound was metabolised (5).

Other comments

Tetrafluoroethylene is considered relatively non-toxic, but can be contaminated at high temperatures with extremely toxic fluorocarbons. The US EPA issued a ruling under section 4 of the Toxic Substances Control Act requiring testing of certain health effects of tetrafluoroethylene (6).

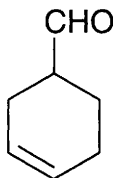
Reviews on human health effects, experimental toxicology and ecotoxicology listed (7).

Inflammable at 14-43% by volume in air (8).

References

1. Odum, J. et al *Toxicol. Appl. Pharmacol.* 1984, **76**(2), 306-318.
2. *Gig. Tr. Prof. Zabol.* 1977, **21**(5), 36.
3. *IARC Monograph* 1987, (Suppl. 7), 72.
4. *National Toxicology Program Research and Testing Division* 1999, Report No. TR-450. NIEHS, Research Triangle Park, NC 27709, USA.
5. Dilley, J. V. et al *Toxicol. Appl. Pharmacol.* 1974, **27**, 582-590.
6. *TSCA Chem. Prog. Bull.* 1987, **4**, 3.
7. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
8. Bikales, N. M. (Ed.) *Encyclopedia of Polymer Science and Technology, Plastics, Resins, Rubbers and Fibers* 1970, **13**, 623-627, Interscience, New York, NY, USA

T71 1,2,3,6-tetrahydrobenzaldehyde



C₇H₁₀O

Mol. Wt. 110.16

CAS Registry No. 100-50-5

Synonyms 4-formylcyclohexene; 3-cyclohexene-1-carboxaldehyde; 1,2,5,6-tetrahydrobenzaldehyde; cyclohexane-4-carboxaldehyde

EINECS No. 202-858-3

RTECS No. GW 2800000

Physical properties

B. Pt. 164°C Flash point 57°C (open cup) Specific gravity 0.940 Volatility v.den. 3.8

Occupational exposure

UN No. 2498 HAZCHEM Code 3  Conveyance classification flammable liquid

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 2460 mg kg⁻¹ (1).

LD₅₀ dermal rabbit 1770 mg kg⁻¹ (1).

Irritancy

Dermal rabbit (24 hr) 10 mg (open) caused mild irritation (1).

Legislation

Recommended for toxicity testing: human health effects, ecological effects and/or subchronic testing under the US Federal Toxic Substances Control Act (2).

References

1. *Am. Ind. Hyg. Assoc. J.* 1962, **23**, 95.
2. *Fed. Regist.* 1991, **56**(44), 9534-9572

T72 tetrahydrofuran



C₄H₈O

Mol. Wt. 72.11

CAS Registry No. 109-99-9

Synonyms diethylene oxide; tetramethylene oxide; THF; oxacyclopentane

EINECS No. 203-726-8

RTECS No. LU 5950000

Uses Solvent for polyvinyl chloride. Solvent in histological techniques. Solvent for resins, adhesives, printers inks and coatings.

Physical properties

M. Pt. -108.5°C B. Pt. 64-66°C Flash point -17°C Specific gravity 0.8892 at 20°C with respect to water at 4°C Partition coefficient log P_{ow} 0.46 Volatility v.p. 131 mmHg at 20°C; v.den. 2.5

Solubility Water: miscible. Organic solvents: miscible with alcohols, esters, ethers, hydrocarbons, ketones

Occupational exposure

DE-MAK 50 ppm (150 mg m⁻³)

FR-VME 200 ppm (590 mg m⁻³)

JP-OEL 200 ppm (590 mg m⁻³)

SE-LEVL 50 ppm (150 mg m⁻³)

UK-LTEL 100 ppm (300 mg m⁻³)

SE-STEL 80 ppm (250 mg m⁻³)

UK-STEL 200 ppm (599 mg m⁻³)

US-TWA 200 ppm (590 mg m⁻³)

US-STEL 250 ppm (737 mg m⁻³)

UN No. 2056 HAZCHEM Code 2YE Conveyance classification flammable liquid

Supply classification highly flammable, irritant

Risk phrases Highly flammable – May form explosive peroxides – Irritating to eyes and respiratory system (R11, R19, R36/37)

Safety phrases Keep out of reach of children (if sold to general public) – Keep away from sources of ignition – No smoking – Do not empty into drains – Take precautionary measures against static discharges (S2, S16, S29, S33)

Ecotoxicity

Fish toxicity

Steelhead trout and sockeye salmon exposed to 10 mg l⁻¹ in a 24 hr static bioassay suffered sickness and loss of equilibrium in 3–4 hr; fatal to sockeye salmon in 16–24 hr. Test conditions: artesian well water, total hardness 67–120 mg l⁻¹; methyl orange alkalinity 151–183 mg l⁻¹; total dissolved solids 160–175 mg l⁻¹ and pH 7.1 (1).

Trout, bluegill sunfish, yellow perch and goldfish exposed to 5 ppm for 24 hr showed no ill-effects. Test conditions: pH 7; dissolved oxygen content 7.5 ppm; total hardness (soap method) 300 ppm; methyl orange alkalinity 310 ppm; free carbon dioxide 5 ppm; at 12.8°C (2).

Invertebrate toxicity

LOEC *Microcystis aeruginosa* 225 mg l⁻¹ reproduction and semichronic studies (duration unspecified) (3).

Cell multiplication inhibition test, toxicity threshold concentration *Uronema parduczi* 858 mg l⁻¹ (4).

Cell multiplication inhibition test *Pseudomonas putida*, inhibition starts at 580 mg l⁻¹ (3).

Cell multiplication inhibition test *Microcystis aeruginosa*, inhibition starts at 225 mg l⁻¹ (3).

Bioaccumulation

No bioaccumulation expected (5).

Environmental fate

Nitrification inhibition

Inhibition of nitrification Agar test limit concentration 360 mg l⁻¹ (6).

Carbonaceous inhibition

Soil microbial respiration was investigated using two slightly acidic soils: a silt loam and a sandy loam. Single 1000 µg g⁻¹ (dry weight) soil, moistened to 80% base saturation and incubated in the dark at 20°C. CO₂ efflux from soils was monitored at 24 hr intervals over a 6-day period. CO₂ efflux increased all days (silt loam) and showed initial decrease followed by later increase (sandy loam) (7).

Degradation studies

Degradation potential was determined using an anaerobic digesting sludge and assessed in terms of net total gas (methane and carbon dioxide) expressed as a percentage of the theoretical production (ThGP). Lag period >60 days, biodegradation potential negative <30% ThGP (8).

1000 mg l⁻¹ was tested using a modified OECD Method 209 Activated Sludge, Respiration Inhibition Test; oxygen consumption rate 94% of control (9).

Confirmed to be biodegradable (10).

Biodegradation tests using activated sludge inoculum, average delay time 17 days; ThOD 0–72% (average 33%) lag time +10 days; after 14 days ThOD 0–63% (average 11%); after 28 days ThOD 0–74% (average 11%) (11).

Abiotic removal

In the atmosphere predicted to degrade with t_{1/2} of hours or days. Rapid degradation is expected, especially under smog conditions. Evaporation is an important environmental fate process from water and soil, t_{1/2} ~90 min. Photodegradation is not expected to occur (5).

No direct photolysation occurs but it will react with hydroxyl radicals in the atmosphere, t_{1/2} 1.6 days (12).

Adsorption and retention

Not expected to adsorb to sediment (5).

Mammalian & avian toxicity

Acute data

LD_{Lo} oral rat 3000 mg kg⁻¹ (13).

LC₅₀ (3 hr) inhalation rat 21,000 ppm (14).

LC₅₀ (4 hr) inhalation mouse 1200 ppm (14).

LD₅₀ intraperitoneal mouse 2500 mg kg⁻¹ (20% olive oil solution) (14).

LD₅₀ intraperitoneal mouse 1900 mg kg⁻¹ (20% of a 0.9% sodium chloride solution) (14).

LD₅₀ intraperitoneal rat 2900 mg kg⁻¹ (20% of a 0.9% sodium chloride solution) (14).

Sub-acute and sub-chronic data

Oral rats (short-term study) lowest dosing solution 1 mg l⁻¹, highest 1000 mg l⁻¹, in drinking water. No overt toxic effects observed at 1000 mg l⁻¹ (duration unspecified) (15).

Inhalation rats, mice (13 wk) 0, 66, 200, 600, 1800 or 5000 ppm. Body weight and survival were not affected, except in ♂ mice exposed to 5000 ppm which had reduced weight and 3 deaths. Clinical signs of central nervous system toxicity were observed in both rats and mice at high-dose levels (16).

Carcinogenicity and chronic effects

The National Toxicology Program tested rats and mice via inhalation. No evidence of carcinogenic activity in ♀ rats and ♂ mice, some evidence of carcinogenicity in ♂ rats, clear evidence of carcinogenicity in ♀ mice (17). Groups of 50 ♂ and ♀ rats and mice were exposed to 200, 600 and 1800 ppm tetrahydrofuran by inhalation 6 hr day⁻¹, 5 days wk⁻¹ for 105 wk. Survival and mean body wt. of exposed rats were comparable with those of controls and no clinical findings or non-neoplastic lesions were observed. Incidence of renal tubule epithelial adenoma or carcinoma occurred with a positive trend in ♂ rats and in animals exposed to ≥600 ppm exceeded the historical range for controls in previous 2 yr inhalation studies. Mean body wt. of ♂ and ♀ mice were similar to those of controls. Survival of ♂ mice exposed to 1800 ppm was significantly lower after 36 wk than controls and animals were in a state of narcosis during and up to 1 hr after exposure. The incidence of hepatocellular neoplasms in ♀ mice exposed to 1800 ppm was significantly greater than in controls (18).

Inhalation rat (20 month) 3000 ppm, 8 hr day⁻¹ no clinical symptoms observed (19).

Teratogenicity and reproductive effects

Inhalation mice, rats exposed to 0, 600, 1800 or 5000 ppm 6 hr day⁻¹ 7 day wk⁻¹ for 6-19 days gestation (rats) and 6-17 days gestation (mice), respectively. Foetal body weights were reduced for animals treated with 5000 ppm, but the incidence of abnormalities was not increased. 95% resorptions occurred in mice given 5000 ppm (20).

Metabolism and toxicokinetics

Following short-term human exposure at concentrations between 100 and 400 ppm, the percentage tetrahydrofuran in expired air was ~35% ♂, ~27% ♀. Following 3 hr exposure, t_{1/2} was ~30 min in alveolar air. After a 6 hr exposure to 50 ppm trace amounts were detected in blood ≤3 hr after exposure (21).

Genotoxicity

In vitro Chinese hamster ovary cells with and without metabolic activation, sister chromatid exchanges and chromosomal aberrations negative (22).

Other effects

Other adverse effects (human)

Skin, eye and mucous membranes irritant. Narcotic at high concentrations (23).

Occupational exposure caused mild effects in the central nervous system, irritation of mucous membranes and cytolytic hepatitis. Subjects had been exposed to high concentrations of the solvent for prolonged periods and all symptoms disappeared within a few hr of cessation of exposure (24).

Legislation

Permitted for use in the USA under the Federal Food, Drug and Cosmetic Act for fabrication of articles for packaging, transporting or storing of foods if the residual amount does not exceed 1.5% of the film (25).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (26).

Other comments

Air pollutant at semiconductor manufacturing plant (27).

Detected in workplace air during the processing of unplasticised PVC (28).

Has been detected in drinking water, ground and surface waters.

Biodegradation with *Bacillus*, *Pseudomonas*, *Micrococcus*, *Arthrobacter* spp. and microorganism selection procedures are discussed (29).

Physical and chemical properties, toxicity, hazards reviewed and French regulations pertinent to its use described (30).

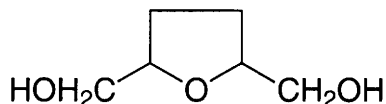
One of a number of chemicals evaluated for toxicity to soil microorganisms, sorption to soil, degradation and potential for bioaccumulation in terrestrial plants and animals (31).

Reviews on human health effects, experimental toxicity, environmental effects, ecotoxicology, epidemiology, workplace experience and physico-chemical properties listed (32).

References

1. *Lethal Effects of 2014 Chemicals Upon Sockeye Salmon, Steelhead Trout and Threespine Stickleback* 1989, US EPA 560/6-89-001, PB 89-156715, Washington, DC, USA.
2. *The Toxicity of 3400 Chemicals to Fish* 1987, EPA 560/6-87-002, PB87-200-275, Washington, DC, USA.
3. Bringmann, G. et al *GWF, Gas-Wasserfach: Wasser/Abwasser* 1976, **117**, 9.
4. Bringmann, G. et al *Z. Wasser/Abwasser Forsch.* 1980, **1**, 26-31.
5. Howard, P. H. *Fate and Exposure Data for Organic Chemicals* 1990, **2**, 430-434, Lewis Publishers, Chelsea, MI, USA.
6. Hansch, C. et al *Med. Chem. Project. Issue No. 26* 1985, Pomona College, Claremont, CA, USA.
7. Walton, B. T. et al *Environ. Toxicol. Chem.* 1989, **8**(1), 53-63.
8. Anderson, T. A. et al *J. Environ. Qual.* 1991, **20**(2), 420-424.
9. Volskay, V. T. et al *J. Water. Pollut. Control Fed.* 1988, **60**(10), 1850-1856.
10. *The list of the existing chemical substances tested on biodegradability by microorganisms or bioaccumulation in fish body* 1987, Chemicals Inspection & Testing Institute, Japan.
11. Doyle, G. J. *Environ. Sci. Technol.* 1975, **9**, 237-241.
12. Winer, A. M. et al *Chem. Phys. Lett.* 1977, **51**, 221-226.
13. *Toksikol. Nov. Prom. Khim. Veshchestv.* 1963, **5**, 21.
14. Horiguchi, S. et al *Seikatsu Eisei* 1991, **35**(3), 137-140.
15. Komsta, E. et al *Bull. Environ. Contam. Toxicol.* 1988, **41**(4), 515-522.
16. Chhabra, R. S. et al *Fundam. Appl. Toxicol.* 1990, **14**(2), 338-345.
17. *National Toxicology Division Research and Testing Division* 1998, Report No. TR 475, NIEHS, Research Triangle Park, NC 27709, USA.
18. Chhabra, R. S. et al *Toxicol. Sci.* 1998, **41**(2), 183-188.
19. Verschuere, K. *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, Van Nostrand Reinhold, New York, NY, USA.
20. Mast, T. J. et al *Fundam. Appl. Toxicol.* 1992, **18**(2), 255-256.
21. Kageyama, M. *Osaka-shi Igakkai Zasshi* 1988, **37**(1), 19-33 (Japan.) (*Chem. Abstr.* **110**, 130128y).
22. Galloway, S. M. et al *Environ. Mol. Mutagen.* 1987, **10**(Suppl. 10), 1-175.
23. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
24. Garnier, R. et al *Br. J. Ind. Med.* 1989, **46**(9), 677-678.
25. *Fed. Reg.* 1962, **27**, 3919.
26. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
27. Yoshida, H. et al *Nippon Sanso Giho* 1988, **7**, 49-55 (Japan.) (*Chem. Abstr.* **112**, 222431m).
28. Barth, E. *Weld. World* 1990, **28**(5-6), 100-103.
29. Dmitrenko, G. N. et al *Khim. Tekhnol. Vody.* 1987, **9**(5), 442-445 (Russ.) (*Chem. Abstr.* **108**, 43260a).
30. *Cah. Notes. Doc.* 1991, **142**, 113-116 (Fr.) (*Chem. Abstr.* **115**, 55787k).
31. Walton, B. T. et al *Report ORNL-6451; DE89016892* 1989, 1-285, NTIS, Springfield, VA, USA.
32. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T73 2,5-tetrahydrofurandimethanol



$C_6H_{12}O_3$

Mol. Wt. 132.16

CAS Registry No. 104-80-3

Synonyms tetrahydrofuran-2,5-diyl dimethanol; THF glycol; 2,5-bis(hydroxymethyl)tetrahydrofuran

EINECS No. 203-239-0

Uses Solvent. Softener. Humectant. Used in the synthesis of plasticisers, resins, surfactants, agricultural chemicals.

Physical properties

M. Pt. $>-50^{\circ}\text{C}$ **B. Pt.** 265°C **Specific gravity** 1.154 at 20°C with respect to water at 4°C

Solubility Water: miscible. Organic solvents: acetone, benzene, chloroform, ethanol, methanol, methyl acetate, methyl ethyl ketone

Occupational exposure

Supply classification irritant

Risk phrases Irritating to eyes, respiratory system and skin (R36/37/38)

Safety phrases Keep out of reach of children (if sold to general public) – Wear eye/face protection (S2, S39)

Other effects

Other adverse effects (human)

Eye, skin and mucous membrane irritant (1).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (2).

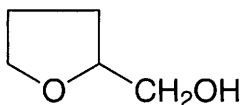
Other comments

Reviews on human health effects, experimental toxicology, ecotoxicology and physico-chemical properties listed (3).

References

1. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
2. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
3. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T74 tetrahydrofurfuryl alcohol



$C_5H_{10}O_2$

Mol. Wt. 102.13

CAS Registry No. 97-99-4

Synonyms tetrahydro-2-furanmethanol; tetrahydro-2-furan carbinol; tetrahydro-2-furylmethanol; THFA

EINECS No. 202-625-6

RTECS No. LU 2450000

Uses Solvent for fats, waxes and resins. Used in organic synthesis.

Physical properties

M. Pt. $<-80^{\circ}\text{C}$ B. Pt. 178°C Flash point 84°C (open cup) Specific gravity 1.0543 at 20°C with respect to water at 20°C Volatility v.p. 2.3 mmHg at 40°C ; v.den. 3.5

Solubility Water: miscible. Organic solvents: acetone, benzene, chloroform, diethyl ether, ethanol

Occupational exposure

Supply classification irritant

Risk phrases Irritating to the eyes (R36)

Safety phrases Keep out of reach of children (if sold to general public) – Wear eye/face protection (S2, S39)

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) harlequin fish 3400 mg l⁻¹ (1).

Bluegill sunfish, trout, yellow perch and goldfish exposed to 5 ppm for 24 hr showed no ill-effects. Test conditions: pH 7.0; dissolved oxygen content 7.5 ppm; total hardness (soap method) 300 ppm; methyl orange alkalinity 310 ppm; free carbon dioxide 5 ppm; and 12.8°C (2).

Environmental fate

Degradation studies

Biodegradation using activated sludge (20°C); tetrahydrofurfuryl alcohol; 96% COD removal at 40 mg COD g⁻¹ dry inoculum hr⁻¹ (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1.6-3.2 g kg⁻¹ (4).

LD₅₀ oral guinea pig 0.8-1.6 g kg⁻¹ (4).

LC₅₀ (6 hr) inhalation rat 12,650 ppm; lowest-observed-no-effect concentration over the 6 hr period 655 ppm (4).

LD_{Lo} intraperitoneal rat 1000 mg kg⁻¹ (5).

LD_{Lo} intravenous rabbit 725 mg kg⁻¹ (6).

Irritancy

100% solution applied to nude mouse skin caused no discernible irritation effects (duration unspecified) (7).

100 µl (undiluted solution) instilled in rabbit eye; ocular irritation recorded at 4, 24, 48, 72, 96 and 168 hr. Not an irritant in Draize test (8).

20 mg instilled into rabbit eye (24 hr) caused moderate to severe irritation (9).

Other effects

Other adverse effects (human)

Moderate irritant to skin and mucous membranes (10).

Other comments

Occurs as D- (CAS RN 22415-59-4) and L- (CAS RN 57203-01-7) isomers.

Reviews on human health effects, experimental toxicology, ecotoxicology and physico-chemical properties listed (11).

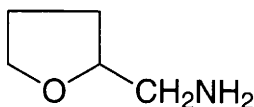
Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (12).

Hygroscopic. Flammable in air: upper limit 9.7% by vol.; lower limit 1.5% by vol.

References

1. Kemp, H. T. et al *Water Quality Data Book, Effects of Chemicals on Aquatic Life* 1973, 5, EPA Water Pollution Control Research Series 09/73.
2. *The Toxicity of 3400 Chemicals to Fish* 1987, EPA560/6-87-002, PB87-200-275, Washington, DC, USA.
3. Pitter, P. *Water Res.* 1976, **10**, 231-235.
4. Patty, F. A. *Industrial Hygiene and Toxicology* 1967, **2**, Interscience Publishers, New York, NY, USA.
5. *J. Pharm. Pharmacol.* 1959, **11**, 150.
6. *Federation Proceedings, Federation of American Societies for Experimental Biology* 1949, **8**, 294.
7. Lashmar, U. T. et al *J. Pharm. Pharmacol.* 1989, **41**(2), 118-122.
8. Jacobs, G. A. et al *ATLA, Altern. Lab. Anim.* 1988, **15**(4), 290-296.
9. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, 138, Prague, Czechoslovakia.
10. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
11. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
12. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T75 tetrahydrofurfuramine



C₅H₁₁NO

Mol. Wt. 101.15

CAS Registry No. 4795-29-3

Synonyms tetrahydro-2-furanmethanamine

EINECS No. 225-351-9

RTECS No. LV 0175000

Physical properties

B. Pt. 153-154°C at 744 mmHg Flash point 45°C Specific gravity 0.980

Occupational exposure

UN No. 2943 HAZCHEM Code 2W Conveyance classification flammable liquid

Ecotoxicity

Fish toxicity

Threespine stickleback, steelhead trout and sockeye salmon exposed to 10 mg l⁻¹ in a 24 hr static bioassay suffered no adverse effects. Test conditions: artesian well water; total hardness 67-120 mg l⁻¹; Methyl Orange alkalinity 151-183 mg l⁻¹; total dissolved solids 160-175 mg l⁻¹ and pH 7 (1).

Mammalian & avian toxicity

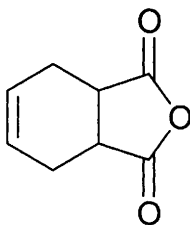
Acute data

LD₅₀ intraperitoneal mouse 200 mg kg⁻¹ (2).

References

1. *Lethal Effects of 2014 Chemicals Upon Sockeye Salmon, Steelhead Trout and Threespine Stickleback* 1989, US EPA560/6-89-001, PB 89-156715, Washington, DC, USA.
2. *NTIS Report AD277-689* Natl. Tech. Inf. Ser., Springfield, VA, USA

T76 tetrahydrophthalic anhydride



C₈H₈O₃

Mol. Wt. 152.15

CAS Registry No. 85-43-8

Synonyms cyclohex-4-ene-1,2-dicarboxylic anhydride; 1,3-isobenzofurandione, 3,4,7,7-tetrahydro-; phthalic anhydride, 1,2,3,6-tetrahydro-; tetrahydrophthalic acid anhydride

EINECS No. 201-605-4

RTECS No. GW 5775000

Uses Analytical chemical reagent for butadiene, polymers.

Physical properties

M. Pt. 101-102°C **B. Pt.** 195°C at 50 mmHg **Flash point** 157°C **Specific gravity** 1.375 at 25°C with respect to water at 20°C **Volatility** v.p. 0.01 mmHg at 20°C; v.den. 5.25

Occupational exposure

UN No. 2698 **HAZCHEM Code** 2Z **Conveyance classification** corrosive substance

Supply classification harmful

Risk phrases Risk of serious damage to eyes – May cause sensitisation by inhalation and skin contact – Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R41, R42/43, R52/53)

Safety phrases Keep out of reach of children (if sold to general public) – Do not breathe dust – Avoid contact with the skin – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Wear suitable gloves and eye/face protection – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S22, S24, S26, S37/39, S61)

Ecotoxicity

Bioaccumulation

No or low bioaccumulation (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 5410 mg kg⁻¹ (2).

LD_{Lo} intraperitoneal mouse 500 mg kg⁻¹ (3).

Irritancy

Dermal rabbit (24 hr) 500 mg caused mild irritation and 20 mg instilled into rabbit eye for 24 hr caused moderate irritation (2).

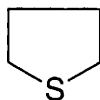
Other comments

Reviews on experimental toxicology and human health effects listed (4).

References

1. JETOC Information Sheet 1992, Jan.-Feb., Japan Chemical Industry Ecology-Toxicology & Information Centre, Nanba Bldg 2F, 19-4, 1-Chome, Nishishinbashi, Minato-Ku, Tokyo, Japan.
2. Marhold, J. V. Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku 1972, 140, Prague, Czechoslovakia.
3. National Research Center Chem. Biol. Coord. Ctr. Summ. Tables. Biol. Texts 1955, 7, 780.
4. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T77 tetrahydrothiophene



C₄H₈S

Mol. Wt. 88.17

CAS Registry No. 110-01-0

Synonyms tetramethylene sulfide; thiacyclopentane; thialane; Thiophane

EINECS No. 203-728-9

RTECS No. XN 0370000

Uses Natural gas odorant.

Occurrence Water pollutant.

Physical properties

M. Pt. -96°C B. Pt. 119°C Flash point 12°C Specific gravity 1.00

Occupational exposure

UN No. 2412 HAZCHEM Code 3WE Conveyance classification flammable liquid

Supply classification highly flammable, harmful

Risk phrases Highly flammable – Harmful by inhalation, in contact with skin and if swallowed – Irritating to eyes and skin (R11, R20/21/22, R36/38)

Safety phrases Keep out of reach of children (if sold to general public) – Keep away from sources of ignition – No smoking – Do not breathe vapour – Wear suitable protective clothing and gloves (S2, S16, S23, S36/37)

Environmental fate

Adsorption and retention

Adsorption and flow in coarse clay, washed river sand, and clay/sand mixture was studied. Breakthrough occurs first in sand and decreases in coarse clay (1).

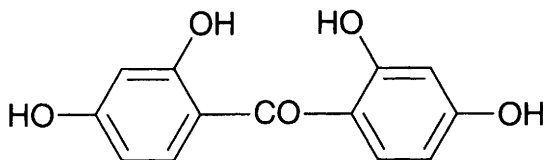
Other comments

Reviews on human health effects, experimental toxicology, ecotoxicology, physico-chemical properties, workplace experience and epidemiology listed (2).

References

1. Palocz, M. et al GWF, *Gas-Wasserfach: Gas/Erdgas* 1987, **128**(2), 60-66 (Ger.) (*Chem. Abstr.* **107**, 179668b).
2. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T78 2,2',4,4'-tetrahydroxybenzophenone



C₁₃H₁₀O₅

Mol. Wt. 255.29

CAS Registry No. 131-55-5

Synonyms bis(2,4-dihydroxyphenyl)methanone; THBP; Uvinol D-50

EINECS No. 205-028-9

RTECS No. DJ 1892000

Uses Ultra-violet absorbing agent used in sunscreens and cosmetics.

Physical properties

M. Pt. 196-198°C

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1220 mg kg⁻¹ (1).

Irritancy

100 mg instilled into rabbit eye for 24 hr caused mild irritation (1).

Genotoxicity

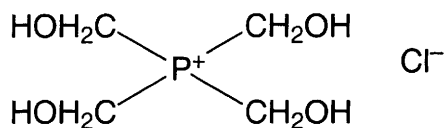
Salmonella typhimurium TA1537 with metabolic activation positive (1,2).

Mouse lymphocyte sister chromatid exchange positive (3).

References

1. *Food Chem. Toxicol.* 1982, **20**, 427.
2. Popkin, D. J. et al *Mutat. Res.* 1989, **224**(4), 453-464.
3. *J. Am. Coll. Toxicol.* 1983, **2**(5), 35

T79 tetrakis(hydroxymethyl)phosphonium chloride



C₄H₁₂ClO₄P

Mol. Wt. 190.56

CAS Registry No. 124-64-1

Synonyms tetrahydroxymethylphosphonium chloride; THPC

EINECS No. 204-707-7

RTECS No. TA 2450000

Uses Production of crease-resistant flame-retardant finishes on cotton textiles and cellulosic fabrics.

Physical properties

M. Pt. 154°C **Flash point** none **Specific gravity** 1.341

Solubility Water: soluble in water

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 400 mg kg⁻¹ (1).

LD_{Lo} intraperitoneal mouse 125 mg kg⁻¹ (2).

LD₅₀ ♂ rat 282 mg kg⁻¹ (3).

Carcinogenicity and chronic effects

Not classifiable as to carcinogenicity to humans, inadequate evidence for carcinogenicity to animals, IARC classification group 3 (4).

The National Toxicology Program tested rats and mice via gavage. No evidence of carcinogenicity in ♂ and ♀ rats and mice (5).

Dermal ♀ mice (420-496 days) dosed three times wk⁻¹ with 2 mg applications. No significant difference in numbers of papillomas of the forestomach and papillary tumours of the lung were found between dosed and control mice (6).

Irritancy

Irritating to rats and rabbits following dermal application (7).

Genotoxicity

Mouse embryo oncogenic transformation system positive at 5000 ppm (8).

Hamster kidney oncogenic transformation system positive at 5000 ppm (8).

Hamster lung cytogenetic analysis positive at 87 mg l⁻¹ (9).

Hamster lung mutation in mammalian somatic cells system 5000 ppm (8).

Salmonella typhimurium TA98, TA100, TA1535, TA1537 negative (10).

Mouse lymphoma L51787 assay (MLA) positive (11).

Chinese hamster ovary cell chromosome aberrations (ABS) positive (11).

Chinese hamster ovary cell induction of chromatid exchanges (SCE) positive (11).

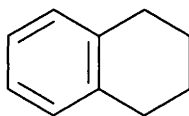
Other comments

Carcinogenic risk to humans reviewed (4).

References

1. Kobunshi. *High Polymers* 1975, **24**, 788.
2. *Summary Tables of Biological Tests* 1955, Vol. 7, p. 789, National Research Council-Biological Coordination Center, National Academy of Science Library, 2101 Constitution Ave., N.W., Washington, DC 20418, USA.
3. Ulsamer, A. G. et al *Clin. Toxicol.* 1980, **17**, 101-131.
4. *IARC Monograph* 1990, **48**, 95-107.
5. *National Toxicology Program Research and Testing Division* 1997, Report No. TR-296, NIEHS, Research Triangle Park, NC 27709, USA.
6. Van Duuren, B. L. et al *Cancer Res.* 1978, **38**(10), 3236-3240.
7. Aoyama, M. *Nagoya Med. J.* 1975, **20**, 11-19.
8. *J. Toxicol. Environ. Health* 1980, **6**, 259.
9. *Gann Monograph on Cancer Research* 1981, **27**, 95.
10. MacGregor, J. T. et al *Environ. Mutagen.* 1980, **2**(3), 405-418.
11. Zeiger, E. et al *Environ. Mol. Mutagen.* 1990, **16**(Suppl 18), 1-14

T80 tetralin



C₁₀H₁₂

Mol. Wt. 132.21

CAS Registry No. 119-64-2

Synonyms 1,2,3,4-tetrahydronaphthalene; Tetranap; $\delta^{5,7,9}$ -naphthantriene; benzocyclohexane

EINECS No. 204-340-2

RTECS No. QK 3850000

Uses Degreasing agent. Solvent for naphthalene, fats, resins, oils and waxes. Used instead of turpentine in lacquers, shoe polishes and floor waxes.

Physical properties

M. Pt. -31°C **B. Pt.** 207.2°C **Flash point** 77°C (open cup); 82°C (closed cup) **Specific gravity** 0.9702 at 20°C with respect to water at 4°C **Volatility** v.p. 0.3 mmHg at 20°C; v.den. 4.55

Solubility Organic solvents: miscible with acetone, benzene, butanol, chloroform, diethyl ether, ethanol, light petroleum

Occupational exposure

Supply classification irritant, dangerous for the environment

Risk phrases May form explosive peroxides – Irritating to eyes and skin – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R19, R36/38, R51/53)

Safety phrases Keep out of reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – After contact with skin, wash immediately with plenty of water – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S26, S28, S61)

Ecotoxicity

Invertebrate toxicity

EC₅₀ (48 hr) *Daphnia pulex* 2.41 mg l⁻¹ at 20°C (1).

Bioaccumulation

Confirmed to be non-accumulative or low accumulative (2).

Environmental fate

Degradation studies

BOD₅ 0% ThOD; ThOD 3.147 (3).

Degradation in seawater by oil-oxidising microorganisms: 31% breakdown after 21 days at 22°C in stoppered bottles containing a 1000 ppm mixture of alkanes, cycloalkanes and aromatics (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 2.86 g kg⁻¹ (5).

LD₅₀ dermal rabbit 17 g kg⁻¹ (6).

Sub-acute and sub-chronic data

Intragastric ♂ ♀ rats (14 day) (unspecified dose every other day) caused renal damage; increased hyaline droplets in proximal convoluted tubular epithelial cells (7).

Metabolism and toxicokinetics

Metabolised in ♂ rats to 1-tetralol, 2-tetralol, 2-hydroxy-1-tetralone, 4-hydroxy-1-tetralone, 1,2-tetralindiol and 1,4-tetralindiol (8).

Irritancy

500 mg applied to rabbit skin (open) caused severe irritation (6).

Genotoxicity

Salmonella typhimurium strains unspecified without metabolic activation negative (9).

Other effects

Other adverse effects (human)

Skin, eye and mucous membrane irritant. Narcotic in high concentrations (10).

Cytological and immunological changes to lymphocytes produced in workers exposed to varnish solvents (11).

Any other adverse effects

Rats treated with 1,2,3,4-tetrahydronaphthalene demonstrated classic lesions of hydrocarbon induced nephropathy (8).

Has produced cataracts in experimental animals (10).

Inhalation of saturated vapours for 8 hr was not lethal to rats (12).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (13).

Other comments

Detected as a pollutant in water.

Listed under the German Chemical Act: reports on hazardous substances detailing environmental fate, ecotoxicity and toxicity have been submitted to the German government (14).

Formation of tetralin peroxide resulting from prolonged exposure to air can cause explosion of tetralin distillation residues. The addition of an antioxidant can prevent peroxide formation (15).

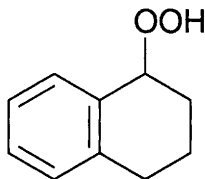
Reviews on human health effects, experimental toxicology, ecotoxicology and physico-chemical properties listed (16).

References

1. Smith, S. B. et al *J. Great Lakes Res.* 1988, **14**(4), 394-404.
2. *The list of the existing chemical substances tested on biodegradability by microorganisms or bioaccumulation in fish body* 1987, Chemicals Inspection & Testing Institute, Japan.

3. Verschueren, K. *The Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, Van Nostrand Reinhold, New York, NY, USA.
4. McKenzie, P. et al *Microbiology in Agriculture, Fisheries and Food* 1976, Skinner, F. A. (Ed.), Academic Press, London, UK.
5. Smyth, et al *Arch. Ind. Hyg. Occup. Med.* 1951, **4**, 119.
6. *Union Carbide Data Sheets* 1972, Union Carbide Corp., New York, NY, USA.
7. Serve, M. P. *Gov. Rep. Announce. Index (U. S.)* 1989, **89**(19), AD-A208588, NTIS, Springfield, VA, USA.
8. Serve, M. P. et al *J. Toxicol. Environ. Health* 1989, **26**(3), 267-275.
9. Jensen, T. E. et al *JAPCA* 1988, **38**(1), 56-58.
10. Browning, E. *Toxicity and Metabolism of Industrial Solvents* 1965, 119-124, Elsevier, New York, NY, USA.
11. Moszczynski, P. et al *Med. Pr.* 1979, **30**(5), 345-352.
12. Pawar, S. S. et al *Ind. J. Biochem. Biophys.* 1975, **12**(2), 133.
13. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
14. Haltrich, W. G. *Vom Wasser* 1989, **73**, 11-24 (Ger.) (*Chem. Abstr.* **112**, 124566q).
15. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
16. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T81 tetralin hydroperoxide



$C_{10}H_{12}O_2$

Mol. Wt. 164.20

CAS Registry No. 771-29-9

Synonyms 1,2,3,4-tetrahydro-1-naphthyl hydroperoxide; tetralyl hydroperoxide

EINECS No. 212-230-0

RTECS No. MX 2625000

Physical properties

M. Pt. 54-56°C Specific gravity 1.098

Occupational exposure

UN No. 2136

Supply classification oxidising, corrosive, dangerous for the environment

Risk phrases May cause fire – Harmful if swallowed – Causes burns – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R7, R22, R34, R50/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep container tightly closed in a cool place – Keep away from acids – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S3/7, S14, S26, S36/37/39, S45, S60, S61)

Ecotoxicity

Invertebrate toxicity

EC₅₀ (72 hr) *Dunaliella bioculata* 0.7 mg l⁻¹ reproductive study (1).

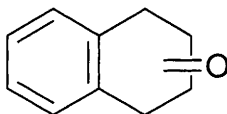
Other comments

Reviews on human health effects and experimental toxicology listed (2).

References

1. Heldal, M. et al *Environ. Pollut. Ser. A* 1984, 35(2), 119-132.
2. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T82 tetralone



$C_{10}H_{10}O$

Mol. Wt. 146.19

CAS Registry No. 29059-07-2

Synonyms 3,4-dihydronaphthalenone; tetralon

EINECS No. 249-394-8

Uses Used in photo-imaging coating.

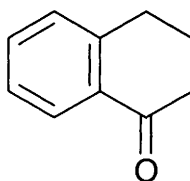
Other comments

Can be converted into ring hydroxylation products by the fungus *Mortierella isabellina* (1).

References

1. Holland, H. L. *Can. J. Chem.* 1987, 65(3), 502-507

T83 α -tetralone



$C_{10}H_{10}O$

Mol. Wt. 146.19

CAS Registry No. 529-34-0

Synonyms 1-oxotetralin; 1-tetralone; 1-oxo-1,2,3,4-tetrahydronaphthalene; 3,4-dihydro-1(2H)-naphthalenone

EINECS No. 208-460-6

RTECS No. QK 4375000

Uses Chemical intermediate. Solvent.

Physical properties

M. Pt. 5.3-6°C **B. Pt.** 113-116°C at 6 mmHg **Flash point** >110°C **Specific gravity** 1.0988 at 16°C with respect to water at 4°C **Volatility** v.p. 0.02 mmHg at 20°C

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird >113 mg kg⁻¹ (2).

LD₅₀ oral rat 810 mg kg⁻¹ (3).

LD₅₀ dermal rabbit >2 g kg⁻¹ (4).

Other comments

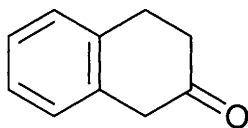
Degradation product of dodecylbenzenesulfonate in activated sludge process (1).

Formed by microbial degradation of 1-naphthol (1).

References

1. Kubodera, T. et al *Yukagaku* 1978, 27(12), 838 (*Chem. Abstr.* 90, 109402m).
2. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, 12, 355-382.
3. *Am. Ind. Hyg. Assoc. J.* 1969, 30, 470.
4. *Toxicol. Appl. Pharmacol.* 1974, 28, 313

T84 β-tetralone



C₁₀H₁₀O

Mol. Wt. 146.19

CAS Registry No. 530-93-8

Synonyms 3,4-dihydro-2(1H)-naphthalenone; 2-tetralone

EINECS No. 208-498-3

Uses Chemical intermediate.

Physical properties

M. Pt. 18°C **B. Pt.** 131°C at 11 mmHg **Flash point** >110°C **Specific gravity** 1.106

Solubility Organic solvents: benzene, diethyl ether

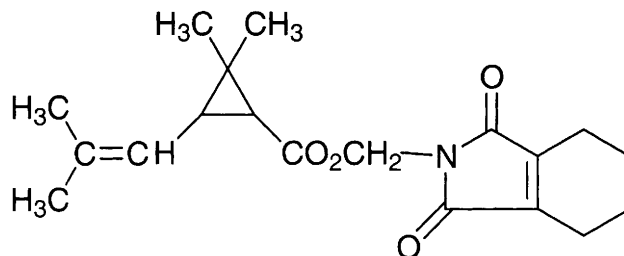
Genotoxicity

Salmonella typhimurium TA98, TA1538, TA100 with and without metabolic activation negative (1).

References

1. McMahon, R. E. et al *Cancer Res.* 1979, 39, 682

T85 tetramethrin



C₁₉H₂₅NO₄

Mol. Wt. 331.41

CAS Registry No. 7696-12-0

Synonyms Neo-Pynamin; 2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylic acid, (1,3,4,5,6,7-hexahydro-1,3-dioxo-2H-isoindol-2-yl) methyl ester; 2,2-dimethyl-3-(2-methylpropenyl)cyclopropanecarboxylic acid ester with *N*-(hydroxymethyl)-1-cyclohexene-1,2-dicarboximide; *N*-(3,4,5,6-tetrahydrophtalimido)methyl *cis*/*trans*-chrysanthemate; *N*-(chrysanthemoxymethyl)-1-cyclohexene-1,2-dicarboximide; phthalthrin

EINECS No. 231-711-6

RTECS No. GZ 1730000

Uses Pyrethroid insecticide, used for indoor pest control.

Physical properties

M. Pt. 65-80°C (technical product ~90% pure) **B. Pt.** 185-190°C at 0.1 mmHg **Specific gravity** 1.108 at 20°C with respect to water at 20°C **Partition coefficient** log *P*_{ow} 4.49 (1) **Volatility** v.p. 7.1 × 10⁻⁶ mmHg at 30°C **Solubility** Water: 4.6 mg l⁻¹ at 30°C. Organic solvents: acetone, benzene, cyclohexanone, ethyl acetate, dichlorodifluoromethane, hexane, kerosene, methanol, methyl isobutyl ketone, methyl naphthalene, piperonyl butoxide, trichloroethane, trichlorofluoromethane, toluene, xylene

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bluegill sunfish 0.021 mg l⁻¹ (1).

LC₅₀ (48 hr) killifish 0.15-0.2 mg l⁻¹ (technical mixture, (+)-*trans*-(+)-*cis*) static bioassay at 25°C (2).

Invertebrate toxicity

LC₅₀ (3 hr) *Daphnia pulex* >50 µg l⁻¹ (technical mixture, (+)-*trans*, (+)-*cis*) static bioassay at 25°C (2).

Toxic to bees (3).

Bioaccumulation

Unlikely to bioaccumulate in organisms (4).

Environmental fate

Degradation studies

Concentrations of 100 mg kg⁻¹ were added to two soil types silt loam and sandy loam soils, t_{1/2} 5.7 day (for abiotic loss and biological degradation) (5).

Environmental degradation involves cleavage of the ester bond, yielding chrysanthemic acid derivatives and phenoxybenzoic acid. Further degradation occurs via hydroxylation and conjugation (1).

Abiotic removal

Following indoor spraying, atmospheric concentrations were 55-300 µg m⁻³. These initial concentrations decreased rapidly due to sedimentation of the aerosol droplets. Levels in surface deposits 15 or 30 min after spraying were measured at 220-900 µg m⁻². Levels were reduced to ~1-10% of the initial amounts after 60 hr. Transformation products detected 12 to 48 hr after spraying were *cis*- and *trans*-tetramethrin (6).

Rapidly degraded when a thin film was exposed to sunlight. The major photoreactions during a 2 hr period (30% conversion) were epoxidation, oxidation and hydroperoxidation (4).

Adsorption and retention

Pyrethroids are strongly adsorbed on soil and sediments, and hardly eluted by water (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat >5000 mg kg⁻¹ (racemic; 1*R*, *cis/trans*) (6,7).

LD₅₀ oral mouse 1000 mg kg⁻¹ (1*R*, *cis/trans*) (7).

LD₅₀ oral rat 4600 mg kg⁻¹ (racemic) (8).

LC₅₀ (3 hr) inhalation rat >2.5 mg l⁻¹ (air) (1).

LD₅₀ dermal rat >5000 mg kg⁻¹ (racemic) >24 hr exposure in corn oil (1).

Sub-acute and sub-chronic data

Oral dog (13 wk) 5000 mg kg⁻¹ (diet) no adverse effects observed; oral rat (6 month) 1500 mg kg⁻¹ (diet) no adverse effects observed (1,4).

Carcinogenicity and chronic effects

Oral rats (104 wk) 0, 200, 1000 and 5000 mg kg⁻¹ diet. No distinct compound-related effects were observed with regard to fertility rate, mortality or clinical signs. However, the highest dose caused lower body-weight gains and increased liver weights. The incidence of interstitial cell tumours was above the level in the concurrent control groups (9).

Teratogenicity and reproductive effects

Oral rats (7-17 days gestation) 0, 100, 300, 1000 mg kg⁻¹ day⁻¹. No abnormalities such as embryo lethality, growth inhibition or teratogenic effects were observed (10).

Metabolism and toxicokinetics

Following a single oral dose of 500 mg kg⁻¹ radiolabelled compound to rats, 47% and 42% of the radiolabel was excreted in the urine and faeces, respectively, within 48 hr and ~95% was metabolised and eliminated via urine and faeces within 5 days. Principal metabolite detected was 3-hydroxycyclohexan-1,2-dicarboximide in free and glucuronide forms (11).

Metabolised in mammals through ester hydrolysis, oxidation and conjugation. There is no tendency for tetramethrin to accumulate in tissues (4).

Irritancy

50 mg instilled into rabbit eye (24 hr) caused transient slight erythema and oedema of the conjunctiva (12).

Dermal rabbit 0.5 ml did not cause irritation (13).

In a semi-closed patch test, an aqueous emulsion containing 1% tetramethrin was applied to the skin of 200 human volunteers for 4 days. 2 wk later a similar application was made. No primary irritation or sensitisation was observed (14).

Sensitisation

Guinea pigs were intracutaneously administered 0.05 ml of a 1% solution in corn oil as the first injection, and subsequently 0.1 ml injections (10 in all over a 20 day period). The animals were then challenged with a 0.5 ml injection 14 days later, but no sensitisation reactions occurred (15).

Genotoxicity

Salmonella typhimurium TA97 without metabolic activation (fluctuation test) positive; without metabolic activation (Ames test) negative (16).

In vitro human peripheral blood lymphocytes chromosomal aberrations positive in agrochemical workers spraying pyrethroids in the open field (17).

In vitro human amniotic cells induced unscheduled DNA synthesis (72% industrial grade tetramethrin). The effect may have been caused by tetramethrin or an unidentified component of the industrial grade material (18).

Other effects

Any other adverse effects

Induced sodium tail current in sodium channel gating mechanism in perfused squid giant axons (19).

Synthetic pyrethroids are neuropoisons affecting the axons in the peripheral and central nervous systems by interacting with sodium channels in mammals and/or insects. A single dose produces toxic signs, including tremors, hyperexcitability, salivation, choreoathetosis and paralysis. Recovery generally takes place within 1 wk (4).

Inhalation rats (3 hr) 0, 26, 131, 243, 595, 1180 mg active ingredient m⁻³ air. Concentrations >131 mg m⁻³ caused salivation, hyperexcitability, irregular respiration, urinary incontinence, muscular fibrillation, limb paralysis in both sexes. The NOEL was 26 mg m⁻³ (20).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (21).

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th amendments) (22).

WHO Toxicity Class Table 5 (23).

EPA Toxicity Class IV (formulation) (3).

Other comments

Chemical structure, biological activity and metabolic pathways reviewed (24).

Chemistry, metabolism, mammalian toxicity and environmental fate reviewed (2,25-28).

Detected in water samples, detection limit 0.01 mg l⁻¹, recovery 91-99%. Degradation products identified were *cis*- and *trans*-dichlorochrysanthemic acid, *cis*- and *trans*-chrysanthemic acid and phthalimide (29).

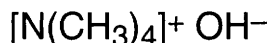
The commercial product is a mixture of 4 stereoisomers: [1*R*,*trans*]; [1*R*,*cis*]; [1*S*,*trans*] and [1*S*,*cis*]. In technical products the composition of isomers is 4:1:4:1. The [1*R*, *trans*] followed by [1*R*, *cis*] are the most biologically active.

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. Miyamoto, J. *Environ. Health Perspect.* 1976, **14**, 15-28.
3. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
4. *Environmental Health Criteria* No. 98: Tetramethrin 1990, WHO, Geneva, Switzerland.
5. Anderson, T. A. et al *J. Environ. Qual.* 1991, **20**(2), 420-424.
6. Kadota, T. et al *Sumitomo Technical Report* No. IT-70-0003 1977, Sumitomo Chemical, Japan.
7. Hiromori, T. et al *Pharmacometrics* 1982, **24**, 179-201.
8. Panshina, T. N. et al *Khim. Selsk. Khoz.* 1983, **12**, 51-53.
9. Pence, D. H. et al *Sumitomo Technical Report* No. IT-11-0097 1981, Sumitomo Chemical, Japan.
10. Sato, T. et al *Sumitomo Technical Report* No. IT-01-0076 1980, Sumitomo Chemical, Japan.
11. Miyamoto, J. et al *J. Agric. Biol. Chem.* 1968, **32**, 628.
12. Okuno, Y. et al *Sumitomo Technical Report* No. IT-60-0013 1976, Sumitomo Chemical, Japan.
13. Hara, S. et al *Sumitomo Technical Report* No. IT-00-0073 1980, Sumitomo Chemical, Japan.
14. Weir, R. J. et al *Sumitomo Technical Report* No. IT-61-0008 1966, Sumitomo Chemical, Japan.
15. Okuno, Y. et al *Sumitomo Technical Report* No. IT-60-0013 1976, Sumitomo Chemical, Japan.
16. Zhang, J. et al *Zhejiang Yike Daxue Xuebao* 1990, **19**(4), 150-153 (Ch.) (*Chem. Abstr.* **114**, 137489h).
17. Nehez, M. et al *Regul. Toxicol. Pharmacol.* 1988, **8**(1), 37-44.
18. Ding, C. et al *Zhejiang Yike Daxue Xuebao* 1985, **14**(1), 1-4.
19. Takeda, K. *Brain Res.* 1988, **448**(2), 308-312.
20. Suzuki, T. et al *Sumitomo Technical Report* No. IT-10-0144 1980, Sumitomo Chemical, Japan.
21. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
22. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
23. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
24. Rozanski, L. *Wiad. Chem.* 1985, **39**(7-8-9), 427-249 (Pol.) (*Chem. Abstr.* **106**, 14245c).
25. Elliot, M. *Synthetic Pyrethroids* 1977, 229, Am. Chem. Soc., Washington, DC, USA.

26. Miyamoto, J. et al *Pesticide chemistry, human welfare and the environment, Proceedings of the Fifth International Congress of Pesticide Chemistry* 1982, 1-4, Pergamon Press, Oxford, UK.
27. Leahey, J. P. *The Pyrethroid Insecticides* 1985, 440, Taylor & Francis Ltd., London, UK.
28. Timofiyevskaya, L. A. et al *Pyrethroids No. 119. Reviews of Scientific Literature in Russian on Selected Hazardous Chemicals* 1993, Engl. Trans. M. L. Richardson, UNEP/IRPTC, Geneva, CIP, Moscow, Russia.
29. Dombek, V. J. *Chromatogr.* 1991, 545(2), 427-435

T86 tetramethylammonium hydroxide



C₄H₁₃NO

Mol. Wt. 91.15

CAS Registry No. 75-59-2

Synonyms *N,N,N*-trimethylmethanaminium hydroxide; methanium hydroxide

EINECS No. 200-882-9

RTECS No. PA 0875000

Uses Chemical reagent, catalyst and intermediate. Developer in lithography and photography.

Physical properties

M. Pt. 63°C (pentahydrate crystals) **Flash point** 37°C **Specific gravity** 1.016 at 25°C with respect to water at 4°C

Occupational exposure

UN No. 1835 **HAZCHEM Code** 2X **Conveyance classification** corrosive substance

Environmental fate

Degradation studies

73 ppm of the compound incubated with anaerobic microorganisms for 85 min can be reduced to <50% of the initial concentration (1).

Protomonas bacteria have been shown capable of degrading the compound (2), as have *Nocardia* species (3).

Mammalian & avian toxicity

Acute data

LD_{Lo} subcutaneous mouse 20 mg kg⁻¹ (4).

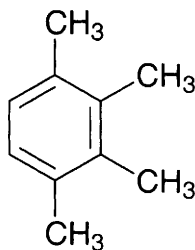
Irritancy

Causes severe burns to skin and eyes and severe irritant damage if ingested (species unspecified) (5).

References

1. Yamazaki, K. et al *Jpn. Kokai Tokkyo Koho* JP63, 270597, 8 November 1988.
2. Uragami, S. et al *Jpn. Kokai Tokkyo Koho* JP01 75,096, 20 March 1989.
3. Oshimi, T. et al *Kogai to Taisaku* 1988, 24(3), 208-212 (Japan.) (*Chem. Abstr.* 108, 226269e).
4. *Arch. Int. Pharmacodyn. Therap.* 1900, 7, 183.
5. *BDH Hazard Data Sheets* 1990, Merck Ltd., Dorset, UK

T87 1,2,3,4-tetramethylbenzene



$C_{10}H_{14}$

Mol. Wt. 134.22

CAS Registry No. 488-23-3

EINECS No. 207-673-1

RTECS No. DC 0465000

Occurrence In crude oil. As a pollutant in lake water (1), seawater (2) and landfill sites (3).

Physical properties

M. Pt. -6°C B. Pt. $204\text{--}205^{\circ}\text{C}$ Flash point 68°C Specific gravity 0.901 Partition coefficient $\log P_{ow}$ 4.00

Solubility Organic solvents: miscible with benzene, diethyl ether, ethanol, light petroleum

Ecotoxicity

Invertebrate toxicity

The water-soluble fraction of Algerian crude oil that contains the compound is toxic to *Phaeodactylum tricornutum* and in turn modifies the feeding behaviour of *Trigriopus brevicornis*, which feeds upon the algae (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 6.4 g kg^{-1} (4).

Irritancy

Dermal rabbit (24 hr) 100 mg caused mild irritation (4).

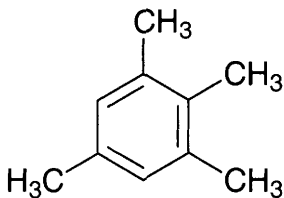
Legislation

The $\log P_{ow}$ value exceeds the European Community recommended level of 3.0 (6th and 7th amendments) (5).

References

1. Juettner, F. Z. *Wasser Abwasser Forsch.* 1988, **21**(2), 36-39.
2. Desideri, P. et al *Ann. Chim. (Rome)* 1989, **79**(11-12), 589-605.
3. Foerst, C. et al *Chemosphere* 1989, **18**(9-10), 1943-1954.
4. *Drug Chem. Toxicol.* 1978, **1**, 219.
5. 1967 Directive on Classification, Packaging and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK

T88 1,2,3,5-tetramethylbenzene



C₁₀H₁₄

Mol. Wt. 134.22

CAS Registry No. 527-53-7

Synonyms isodurene

EINECS No. 208-417-1

RTECS No. DC 0475000

Occurrence Occurs in coal tar and crude oil. As a pollutant in lake water (1).

Physical properties

M. Pt. -24°C B. Pt. 197.9°C Specific gravity 0.8961 at 0°C with respect to water at 4°C

Partition coefficient log P_{ow} 4.10

Solubility Organic solvents: diethyl ether, ethanol

Ecotoxicity

Invertebrate toxicity

The water-soluble fraction of Algerian crude oil that contains the compound is toxic to *Phaeodactylum tricornutum* and in turn modifies the feeding behaviour of *Trigriopus brevicornis*, which feeds upon the algae (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 5.157 g kg⁻¹ (2).

Irritancy

Dermal rabbit (24 hr) 100 mg caused mild irritation (2).

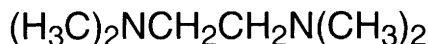
Legislation

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th amendments) (3).

References

1. Juettner, F. Z. *Wasser Abwasser Forsch.* 1988, **21**(2), 36-39.
2. *Drug Chem. Toxicol.* 1978, **1**, 219.
3. 1967 Directive on Classification, Packaging and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK

T89 ***N,N,N',N'*-tetramethylethylenediamine**



$\text{C}_6\text{H}_{16}\text{N}_2$

Mol. Wt. 116.21

CAS Registry No. 110-18-9

Synonyms *N,N,N',N'*-tetramethyl-1,2-ethanediamine; 1,2-bis(dimethylamino)ethane; propamine D; Temed

EINECS No. 203-744-6

RTECS No. KV 7175000

Uses Chemical intermediate.

Physical properties

M. Pt. -55°C B. Pt. 122°C Flash point 10°C Specific gravity 0.77

Solubility Water: miscible

Occupational exposure

UN No. 2372 HAZCHEM Code 3WE Conveyance classification flammable liquid

Supply classification highly flammable, corrosive

Risk phrases Highly flammable – Harmful by inhalation and if swallowed – Causes burns (R11, R20/22, R34)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep away from sources of ignition – No smoking – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S16, S26, S36/37/39, S45)

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird 96-100 mg kg⁻¹ (1).

LD₅₀ dermal rabbit 5.4 g kg⁻¹ (2).

Irritancy

10 mg applied unoccluded to rabbit skin caused irritation (duration unspecified) (3).

750 µg applied to rabbit eye caused severe irritation (4).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (5).

Other effects

Other adverse effects (human)

Irritant to the respiratory system (6).

Any other adverse effects

Biochemical actions include effects on gamma-glutamyl transferase activity in cultured rat cortical astroglial cells (7) and effects on saccharide and phospholipid concentrations in cultured rabbit aorta cells (8).

Other comments

Environmental pollutant.

Toxicity has been reviewed and a safe concentration in reservoir water has been proposed as 0.5 mg l⁻¹ (9).

References

1. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
2. *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 470.

3. *J. Ind. Hyg. Toxicol.* 1948, **30**, 63.
4. *Am. J. Ophthalmol.* 1946, **29**, 1363.
5. Zeiger, E. et al *Environ. Mol. Mutagen.* 1987, **9**(9), 1-109.
6. *BDH Hazard Data Sheets* 1990, Merck Ltd.
7. Seiler, N. et al *Neurochem. Res.* 1990, **15**(3), 301-305.
8. Zadok, R. et al *Lab. Invest.* 1991, **64**(4), 574-584.
9. Shtabskii, B. et al *Gig. Sanit.* 1991, (8), 80-81 (Russ.) (*Chem. Abstr.* 115, 225766x)

T90 tetramethyllead



$\text{C}_4\text{H}_{12}\text{Pb}$

Mol. Wt. 267.34

CAS Registry No. 75-74-1

Synonyms lead tetramethyl; tetramethylplumbane

EINECS No. 200-897-0

RTECS No. TP 4725000

Uses Component of anti-knock mixes for motor petrol.

Physical properties

M. Pt. -27.8°C B. Pt. 110°C (decomp.) Flash point 37.8°C Specific gravity 1.99 Volatility v.den. 9.2
Solubility Water: 15 mg l⁻¹ seawater. Organic solvents: benzene, diethyl ether, ethanol

Occupational exposure

DE-MAK 0.05 mg m⁻³ (as Pb)

FR-VME 0.15 mg m⁻³ (as Pb)

SE-LEVL 0.05 mg m⁻³ (as Pb)

SE-STEL 0.2 mg m⁻³ (as Pb)

UK-LTEL 0.15 mg m⁻³ (as Pb)

US-TWA 0.15 mg m⁻³ (as Pb)

UN No. 1649 HAZCHEM Code 2WE Conveyance classification toxic substance

Supply classification very toxic

Risk phrases May cause harm to the unborn child – Possible risk of impaired fertility – Very toxic by inhalation, in contact with skin and if swallowed – Danger of cumulative effects (R61, R62, R26/27/28, R33)

Safety phrases Restricted to professional users – Avoid exposure – obtain special instruction before use – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S53, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) bass 0.10 mg l⁻¹ static bioassay at 20°C (1).

LC₅₀ (96 hr) tidewater silverside, bluegill sunfish, 13.5-84 mg l⁻¹, (static bioassay), pH 7.6-7.9, hardness 55 mg l⁻¹ (CaCO₃) and temperature 20-23°C (2).

LC₅₀ (96 hr) plaice 0.05 mg l⁻¹ flow-through bioassay at 15°C and 34.9 mg l⁻¹ (CaCO₃) salinity (3).

Invertebrate toxicity

Scenedesmus quadricauda, *Ankistrodesmus falcatus* and *Chlorella pyrenoidosa* (7 day) <0.5 mg decrease in growth 32, 32 and 74%, respectively. Tetramethyllead is 2 × as toxic as trimethyllead acetate and 20 × as toxic as lead nitrate for the same organisms (4).

LC₅₀ (96 hr) mussel, brown shrimp 0.27 mg l⁻¹ and 0.11 mg l⁻¹, (flowthrough bioassay) at 15°C and 34.9% salinity (3).

It is non-toxic to freshwater and marine algae (duration and concentration unspecified). The trialkyllead degradation product is responsible for the apparent toxicity of tetramethyllead (5).

Bioaccumulation

In Canada, northern pike and redhorse sucker living in rivers near alkyllead production plants contained 0.17 and 5 $\mu\text{g g}^{-1}$, respectively (6).

Accumulation (96 hr) in shrimp at 0.11 mg l^{-1} gave a concentration factor of 20 (7).

Accumulation (96 hr) *Mytilus edulis* at 0.27 mg l^{-1} gave a mean concentration factor of 170 for digestive gland, foot, gill and gonads (7).

Accumulation (96 hr) plaice at 0.05 mg l^{-1} gave a concentration factor of 60 (7).

Environmental fate

Degradation studies

BOD using mixed coastal marine bacteria, concentrations $<3.2 \text{ mg l}^{-1}$ O_2 did not effect the lag phase significantly.

EC_{50} (48 hr) 1.9 mg l^{-1} (1).

EC_{50} (48 hr) *Dunaliella tertiolecta* 1.65 mg l^{-1} (1).

Mammalian & avian toxicity

Acute data

LD_{50} oral rabbit, rat 24, 105 mg kg^{-1} , respectively (8,9).

LD_{Lo} dermal rabbit 3391 mg kg^{-1} (9).

LD_{50} intraperitoneal rat 90 mg kg^{-1} (8).

LD_{50} intravenous rat, rabbit 88-90 mg kg^{-1} (8,10).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (11).

Teratogenicity and reproductive effects

Oral Simonsen Sprague-Dawley rats 40, 80, 112 or 160 mg kg^{-1} on 3 consecutive days (9, 10, 11 or 12, 13, 14) of organogenesis. Doses up to those lethal to some mother animals were essentially non-teratogenic to offspring (7).

Metabolism and toxicokinetics

Intravenous (7 day) rabbit 9.9 or 39.7 mg kg^{-1} . Urinary total lead excretion for 9.9 mg kg^{-1} was 73% dimethyllead, 19% trimethyllead, 6% inorganic lead and 2% tetramethyllead on the day following the injection, and 100% trimethyllead 7 days after the injection. For 39.7 mg kg^{-1} the urinary total lead excretion was 67% dimethyllead, 14% trimethyllead, 17% inorganic lead and 2% tetramethyllead on the day following the injection, and 8% dimethyllead, 74% trimethyllead, 17% inorganic lead and 1% tetramethyllead 7 days after the injection. Faecal total lead excretion for the 7 days was composed of 100% inorganic lead. During the 7 days 1-3% of either administered dose was excreted in the urine and 7-19% in the faeces (12).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (13).

Other comments

Organolead compounds are generally 10-100 \times more toxic to aquatic organisms than inorganic leads.

Tetraalkyllead becomes toxic by conversion into trialkyllead (14).

Detected in soils and organisms close to roads with high traffic density.

Lead from tetramethyllead in soil and vegetation decreases exponentially with the distance from the road. Levels in plants and animals increase in areas close to roads; the levels are positively correlated with traffic volume and proximity of roads (14).

Tetramethyllead was produced from inorganic lead salts using biologically active sediments and estuarine waters. Tetramethyllead formation was a two-stage process involving an initial lag of ~ 100 hr followed by the exponential appearance of tetramethyllead which amounted to $\sim 0.03\%$ of total added lead (15).

Tetraalkyllead compounds are the predominant alkyllead compounds in the atmosphere. They are removed from the air in rainwater and transferred to surface and highway drainage water; sequential breakdown of tetraalkyllead to tri- and dialkyllead compounds occurs (16). Tetramethyllead is not soluble in water and is volatile.

References

1. Marchetti, R. *Mar. Pollut. Bull.* 1978, **9**, 206-207.
2. Dawson, G. W. et al *J. Hazard. Mater.* 1977, **1**, 303-318.
3. Maddock, B. G. et al *Lead in the Marine Environment* 1980, 233-261, Pergamon Press, Oxford, UK.
4. Silverberg, B. A. et al *Arch. Environ. Contam. Toxicol.* 1977, **5**, 305-313.
5. Jarvie, A. W. P. *Appl. Organomet. Chem.* 1987, **1**(1), 29-38.
6. Chau, Y. K. et al *Chem. Environ. Proc. Int. Conf.* 1986, 77-82.
7. McClain, R. M. et al *Toxicol. Appl. Pharmacol.* 1972, **21**, 265-274.
8. *Ind. Med.* 1963, **54**, 486.
9. *Jpn. J. Ind. Health* 1973, **15**, 3.
10. *J. Pharmacol. Exp. Ther.* 1930, **38**, 161.
11. *IARC Monograph* 1987, **Suppl. 7**, 230-232.
12. Arai, F. et al *Ind. Health* 1990, **28**(2), 63-76.
13. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
14. *IPCS Environmental Health Criteria 85: Lead – Environmental Aspects* 1989, WHO, Geneva, Switzerland.
15. Walton, A. P. et al *Appl. Organomet. Chem.* 1988, **2**(1), 87-90.
16. Radojevic, M. *Heavy Met. Environ., Int. Conf. 5th* 1985, **1**, 82-84

T91 tetramethyl orthosilicate



$\text{C}_4\text{H}_{12}\text{O}_4\text{Si}$

Mol. Wt. 152.22

CAS Registry No. 681-84-5

Synonyms silicic acid, tetramethyl ester; methyl orthosilicate; tetramethyl silicate; silicon methoxide; TMOS; tetramethoxysilane

EINECS No. 211-656-4

RTECS No. VV 9800000

Physical properties

M. Pt. -4°C B. Pt. $121\text{--}122^\circ\text{C}$ Flash point 28°C Specific gravity 1.032 Volatility v.p. 760 mm Hg at 121°C ; v.den. 5.25

Occupational exposure

FR-VME 1 ppm (6 mg m^{-3})

JP-OEL 1 ppm (6 mg m^{-3})

UK-LTEL 1 ppm (6.3 mg m^{-3})

UK-STEEL 5 ppm (32 mg m^{-3})

US-TWA 1 ppm (6 mg m^{-3})

UN No. 2606 HAZCHEM Code 3WE Conveyance classification toxic substance, danger of fire (flammable liquid)

Mammalian & avian toxicity

Acute data

LC_{Lo} (4 hr) inhalation rat 250 ppm (1).

LD₅₀ dermal rabbit 17 g kg⁻¹ (1).

LD₅₀ intraperitoneal mouse 250 mg kg⁻¹ (2).

Sub-acute and sub-chronic data

Inhalation rats (28 day) 0, 1, 5 and 10 ppm (phase I study) and 0, 15, 30 and 45 ppm (phase II study) 6 hr day⁻¹, 5 day wk⁻¹. All rats exposed to 45 ppm died within 28 days. Statistically significant changes were observed in food consumption, body-weight gains and clinical chemistry parameters in the animals exposed to 30 ppm. ♂ exposed to 15 ppm showed significant decrease in total protein. Histopathological lesions, ulceration, inflammation and necrosis of epithelium were observed in the respiratory tract tissues and eyes of rats exposed to 15, 30 and 45 ppm. No effects were seen in rats exposed to 1, 5 and 10 ppm (3).

Irritancy

250 µg instilled into rabbit eye (open) caused severe irritation (duration unspecified) (1).

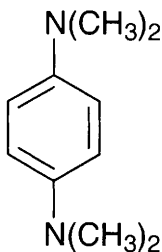
Other comments

Reviews on human health effects, experimental toxicology, environmental effects and workplace experience listed (4).

References

1. AMA, *Arch. Ind. Hyg. Occup. Med.* 1951, **4** 119.
2. *Summary Tables of Biological Tests* 1950, **2**, 56, Natl. Res. Cn. Chem. Biol. Coord. Cent., Washington, DC, USA.
3. Kolesar, G. B. et al *Fundam. Appl. Toxicol.* 1989, **13**(2), 285-295.
4. ECETOC *Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T92 *N,N,N',N'*-tetramethyl-*p*-phenylenediamine



C₁₀H₁₆N₂

Mol. Wt. 164.25

CAS Registry No. 100-22-1

Synonyms *N,N,N',N'*-tetramethyl-1,4-benzenediamine; TMPD; *p*-bis(dimethylamine)benzene; Wurster's reagent; Wurster's blue

EINECS No. 202-831-6

RTECS No. ST 4200000

Uses Photochemical reactant. Chemical reagent. Antioxidant.

Physical properties

M. Pt. 49-51°C B. Pt. 260°C Flash point >100°C

Solubility Organic solvents: diethyl ether, ethanol

Occupational exposure

Supply classification harmful

Risk phrases Harmful by inhalation, in contact with skin and if swallowed (R20/21/22)

Safety phrases Keep out of reach of children (if sold to general public) – After contact with skin, wash immediately with plenty of water (S2, S28)

Mammalian & avian toxicity

Acute data

LD_{Lo} oral rat 500 mg kg⁻¹ (1).

LC_{Lo} (10 min) inhalation mouse 780 mg m⁻³ (2).

Carcinogenicity and chronic effects

Rats given a single dose of 7,12-dimethylbenzanthracene and subsequently fed a diet containing 1% N,N,N',N'-tetramethyl-p-phenylenediamine developed a reduced number of fibroadenomas compared with those fed a control diet (3).

Genotoxicity

Salmonella typhimurium TA97, TA100 with and without metabolic activation positive (4).

In vitro Chinese hamster lung cells (24 and 48 hr) without metabolic activation positive, with metabolic activation weakly positive. Chinese hamster ovary cells without metabolic activation weakly positive, with metabolic activation positive (5).

Other effects

Any other adverse effects

In rats, muscle necrosis occurs in a manner consistent with the production of free radicals seen *in vitro* (6).

The compound reduces cytochrome c *in vitro* (7).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (8).

References

1. J. Pharm. Exp. Therap. 1947, **90**, 260.
2. Nat. Def. Res. Committee (U.S.) **132**, December 1942.
3. Masanda, A. et al *Nagoya-Shiritsu Daigaku Igakkai Zasshi* 1988, **39**(2), 365-386 (Japan.) (*Chem. Abstr.* **109**, 183170t).
4. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-157.
5. Sofuni, T. et al *Mutat. Res.* 1990, **241**(2), 175-213.
6. Munday, R. et al *Toxicology* 1989, **57**(3), 303-314.
7. Cokic, P. et al *Biochim. Biophys. Acta* 1987, **913**(3), 257-271.
8. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T93 tetramethylsilane



$\text{C}_4\text{H}_{12}\text{Si}$

Mol. Wt. 88.22

CAS Registry No. 75-76-3

EINECS No. 200-899-1

Uses Chemical intermediate, anti-knocking agent, and in protective coatings.

Physical properties

M. Pt. -99°C B. Pt. -27°C Flash point -27°C Specific gravity 0.648 Volatility v.p. 560 mmHg at 20°C

Occupational exposure

UN No. 2749 HAZCHEM Code 3WE Conveyance classification flammable liquid

Environmental fate

Abiotic removal

The degree of photolytic degradation by ozone suggests that the compound will not accumulate in the atmosphere. Degradation is accelerated by water (1).

Mammalian & avian toxicity

Irritancy

May be irritating to eyes and the respiratory system (species unspecified) (2).

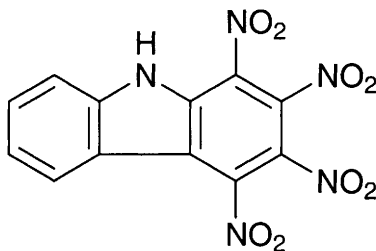
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (3).

References

1. Abe, Y. et al *J. Macromol. Sci. Chem.* 1981, **A16**(2), 461-467.
2. *BDH Hazard Data Sheets* 1990, Merck Ltd.
3. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T94 1,2,3,4-tetranitrocarbazole



$C_{12}H_5N_5O_8$

Mol. Wt. 347.20

CAS Registry No. 6202-15-9

Occupational exposure

Supply classification explosive, harmful

Risk phrases Explosive when dry – Harmful by inhalation, in contact with skin and if swallowed (R1, R20/21/22)

Safety phrases Keep out of reach of children (if sold to general public) – This material and its container must be disposed of in a safe way (S2, S35)

Other comments

The compound may contribute to the mutagenicity of carbazole when exposed to NO_2 and irradiation by light and tested without metabolic activation using *Salmonella typhimurium* TA98 (1).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (2).

References

1. Hisamatsu, Y. et al *Mutat. Res.* 1989, **226**(1), 55-59.
2. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T95 tetranitromethane



CN_4O_8

Mol. Wt. 196.03

CAS Registry No. 509-14-8

Synonyms TNM

EINECS No. 208-094-7

RTECS No. PB 4025000

Occurrence Occurs as an impurity in TNT.

Physical properties

M. Pt. 13.8°C **B. Pt.** 126°C **Flash point** >110°C **Specific gravity** 1.623 at 25°C with respect to water at 4°C

Volatility v.p. 10 mmHg at 22.7°C; v.den. 6.8

Solubility Water: 90 mg l⁻¹ at 20°C. Organic solvents: diethyl ether, ethanol

Occupational exposure

FR-VME 1 ppm (8 mg m⁻³)

SE-LEVL 0.05 ppm (0.4 mg m⁻³)

US-TWA 0.005 ppm (0.04 mg m⁻³)

SE-STEL 0.1 ppm (0.8 mg m⁻³)

UN No. 1510 HAZCHEM Code 2WE Conveyance classification oxidising substance, toxic

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 130 mg kg⁻¹ (1).

LD₅₀ oral mouse 375 mg kg⁻¹ (1).

LC₅₀ (4 hr) inhalation rat 18 ppm (2).

LD₅₀ intravenous rat 12.6 mg kg⁻¹ (2).

LD₅₀ intravenous mouse 63 mg kg⁻¹ (2).

Carcinogenicity and chronic effects

National Toxicology Program tested rats and mice by inhalation of 0.5-5 ppm, 6 hr day⁻¹, 5 days wk⁻¹ for 2 yr. Clear evidence of carcinogenicity was seen in both species. ♀ rats and ♀ and ♂ mice showed increased incidence of alveolar and bronchiolar neoplasms while ♂ rats showed hyperplasia and squamous cell metaplasia of respiratory epithelium. Irritation of nasal passages was observed (3,4).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA102 with and without metabolic activation positive (5).

Other effects

Any other adverse effects

The compound is a nitrosating agent and nitrosation at bovine muscarinic and dopaminergic receptors *in vitro* can modify ligand binding at these sites. Nitrosation of tyrosine residues is thought to be particularly important (6,7).

Other comments

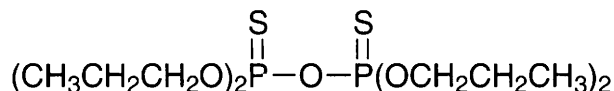
Chemical reagent. Oxidiser in rocket propellants.

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (8).

References

1. NTIS Report AD-A051-334, Natl. Tech. Inf. Ser., Springfield, VA, USA.
2. *Aerospace Med. Res. Rep.* TR-77-25-77.
3. Bucher, J. R. *Cancer Lett. (Shannon, Irel.)* 1991, **57**(2), 95-101.
4. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-386, NIEHS, Research Triangle Park, NC, USA.
5. Wuergler, F. G. et al *Mutat. Res.* 1990, **244**(1), 7-14.
6. Yamanaka, K. et al *Jpn. J. Pharmacol.* 1988, **48**(1), 67-76.
7. Srivastava, L. K. *Biochem. Int.* 1990, **21**(4), 705-714.
8. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T96 tetrapropyl dithiopyrophosphate



$\text{C}_{12}\text{H}_{28}\text{O}_5\text{P}_2\text{S}_2$

Mol. Wt. 378.43

CAS Registry No. 3244-90-4

Synonyms *O,O,O,O*-tetrapropyl dithiopyrophosphate; bis(*O,O*-dipropyl) phosphorothionic anhydride; propyl thiopyrophosphate; Aspon

EINECS No. 221-817-0

RTECS No. XN 4550000

Uses Superseded non-systemic insecticide.

Physical properties

M. Pt. -45°C **B. Pt.** $\sim 170^\circ\text{C}$ at 1 mmHg **Specific gravity** 1.12 at 20°C with respect to water at 20°C

Volatility v.p. $\sim 9.7 \times 10^{-5}$ mmHg at 25°C

Solubility Water: 30 mg l^{-1} at 20°C . Organic solvents: miscible with acetone, ethanol

Occupational exposure

Supply classification harmful, dangerous for the environment

Risk phrases Harmful in contact with skin and if swallowed – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R21/22, R50/53)

Safety phrases Keep out of reach of children (if sold to general public) – Wear suitable protective clothing and gloves – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S36/37, S60, S61)

Environmental fate

Degradation studies

The compound is persistent in soil (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral chicken 436 mg kg^{-1} (2).

LD₅₀ oral redwing blackbird, starling 100 mg kg^{-1} (3).

LD₅₀ oral rat 450 mg kg^{-1} (4).

LD₅₀ dermal rat 1.8 g kg^{-1} (5).

LD₅₀ intraperitoneal mouse 8 mg kg^{-1} (6).

LD₅₀ intravenous mouse 3.25 mg kg^{-1} (6).

Irritancy

Mildly irritating to skin, non-irritating to eyes of rabbits (1).

Genotoxicity

Salmonella typhimurium CASE (computer automated structure evaluation) study predicted mutagenic activity (7).

Other effects

Any other adverse effects

In a 90-day feeding trial in rats, non-lethal doses reduced values of red blood cell cholinesterase (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (8).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (9).

References

1. *The Pesticide Manual* 8th ed., 1987, British Crop Protection Council, Farnham, UK.
2. *Toxicol. Appl. Pharmacol.* 1964, **6**, 147.
3. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
4. *World Rev. Pest Control* 1970, **9**, 119.
5. *Toxicol. Appl. Pharmacol.* 1960, **2**, 88.
6. *Can. J. Chem.* 1956, **34**, 1819.
7. Klopman, G. et al *Mutat. Res.* 1990, **228**(1), 1-50.
8. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
9. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T97 tetrapropyl orthotitanate



C₁₂H₂₈O₄Ti

Mol. Wt. 284.23

CAS Registry No. 3087-37-4

Synonyms titanium(IV) propoxide

EINECS No. 221-411-3

Uses Chemical intermediate, catalyst, in heat resistant surface coatings.

Physical properties

B. Pt. 170°C at 3 mmHg **Flash point** 42°C **Specific gravity** 1.033

Occupational exposure

UN No. 2413 **HAZCHEM Code** 2YE **Conveyance classification** flammable liquid

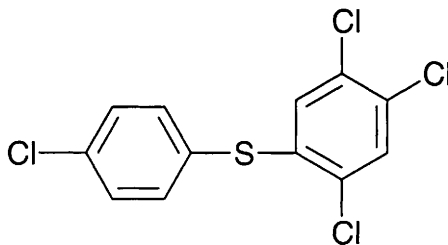
Mammalian & avian toxicity

Metabolism and toxicokinetics

Titanium compounds are not normally absorbed from the gastro-intestinal tract of mammals. There are no reported mechanisms for titanium detoxification (1).

References

1. Venugopal, B. et al *Metal Toxicity in Mammals* 2 1978, Plenum Press, New York, NY, USA

**C₁₂H₆Cl₄S****Mol. Wt.** 324.06**CAS Registry No.** 2227-13-6

Synonyms *p*-chlorophenyl-2,4,5-trichlorophenyl sulfide; 4-chlorophenyl 2,4,5-trichlorophenyl sulfide; 1,2,4-trichloro-5-[(4-chlorophenyl)thio]benzene; Animert; Philips-Duphar U-101

EINECS No. 218-761-4**RTECS No.** WQ 3850000

Uses Superseded, non-systemic acaricide.

Physical properties

M. Pt. 88.4-88.6°C **Volatility** v.p. 7.52×10^{-7} mmHg at 20°C

Solubility Water: 0.03 mg l⁻¹ at 20°C. Organic solvents: ethanol, xylene

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) rainbow trout, goldfish, black bullhead and bluegill sunfish >10 mg l⁻¹ (1).

Invertebrate toxicity

Non-toxic to bees (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 3.96 g kg⁻¹ (2).

LD₅₀ oral mouse 5.01 g kg⁻¹ (3).

LD₅₀ oral guinea pig 500 mg kg⁻¹ (4).

LD₅₀ dermal rabbit >2 g kg⁻¹ (1).

LD₅₀ intraperitoneal guinea pig 550 mg kg⁻¹ (4).

Sub-acute and sub-chronic data

In a 90-day feeding trial beagle dogs tolerated a dose of 200 mg kg⁻¹ diet (1).

LC₅₀ (8 day) bobwhite quail 1.2 g kg⁻¹ diet (1).

Carcinogenicity and chronic effects

A 2-yr feeding trial in rats established a NOEL of 10 mg kg⁻¹ diet (1).

Teratogenicity and reproductive effects

A three-generation study in rats established a NOEL of 20 mg kg⁻¹ diet (1).

Legislation

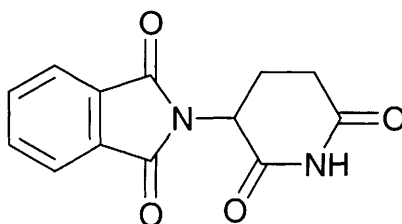
Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (5).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (6).

References

1. *The Pesticide Manual* 8th ed., 1987, British Crop Protection Council, Farnham, UK.
2. *Bull. Entomol. Soc. America* 1969, **15**, 129.
3. *Guide to Chemicals used in Crop Protection* 1973, **6**, 495.
4. *Toxicology* 1973, **1**, 63.
5. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
6. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T99 thalidomide



$C_{13}H_{10}N_2O_4$

Mol. Wt. 258.23

CAS Registry No. 50-35-1

Synonyms 2-(2,6-dioxo-3-piperidiny)-1*H*-iso-indole-1,3(2*H*)-dione; *N*-phthaloylglutarimide; *N*-(2,6-dioxo-3-piperidiny)phthalamide; 2-phthalimidoglutarimide; NSC-66847; Kevadon; K-17

EINECS No. 200-031-1

RTECS No. TI 4375000

Uses Hypnotic, no longer in general use as such. Experimental therapeutic use as an immunosuppressant for a variety of infections and conditions, including leprosy, HIV infection and transplant rejection (1-3).

Physical properties

M. Pt. 269-271°C

Solubility Water: sparingly soluble. Organic solvents: dimethylformamide, 1,4-dioxane, pyridine

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 2 g kg⁻¹ (4).

The compound has a variety of central nervous system depressant effects, including sedation and potentiation of sleeping time in mice (5).

Teratogenicity and reproductive effects

Teratogenic effects have been extensively studied and confirmed in experimental animals following the human foetal abnormalities reported in the early 1960s (6-10).

Metabolism and toxicokinetics

♂ Volunteers receiving an oral dose of 200 mg developed a peak plasma concentration after 4.4 hr; *t*_{1/2} was 8.7 hr. Urinary excretion was only 0.6% of dose over 24 hr, indicating that the major route of metabolism was non-renal (11).

An arene oxide metabolic intermediate is thought to be responsible for some of the adverse effects (12,13).

The relevance of chirality in metabolism and toxicity has been reviewed (9).

Genotoxicity

Dominant lethal assay mice using an intraperitoneal dose of 0.8-1.6 g kg⁻¹ negative (14). *Salmonella typhimurium* six tester strains with and without metabolic activation negative. Non-clastogenic in cultured human lymphocytes and Chinese hamster ovary cells treated *in vitro*. No induction of micronuclei in isolated human lymphocytes without metabolic activation. No indication of recombinogenic or clastogenic activity in *Drosophila melanogaster*. Thalidomide is neither a mutagen nor an aneugen (15).

Other effects

Other adverse effects (human)

Teratogenic effects led to the withdrawal of the drug from general use in the 1960s. These effects involved malformations of limbs, along with defects of eyes, ears and internal organs. The incidence of central nervous system effects was particularly high, due to use of the drug as an antiemetic in the early weeks of pregnancy. The other major adverse effect seen in patients taking the drug was peripheral neuropathy. Other side-effects include constipation, peripheral oedema and dryness of the mouth and nasal mucosa (10,16).

Any other adverse effects

The compound lowers hepatic levels of NADH and NADPH in pregnant rats and their foetuses (17).

Other comments

Lack of mutagenic activity across phyla and genetic endpoints and possibility that thalidomide may be a heritable germ cell mutagen to humans discussed (15).

References

1. Sheskin, J. *Int. J. Dermatol.* 1980, **19**, 318.
2. Youle, M. et al *Br. Med. J.* 1989, **298**, 432.
3. Lim, S. H. et al *Lancet* 1988, **i**, 117.
4. *Life Sci.* 1964, **3**, 721.
5. Buech, H. P. et al *Arzneim.-Forsch.* 1990, **40**(1), 32-36 (Ger.) (*Chem. Abstr.* **113**, 17466f).
6. Fratta, I. D. *Toxicol. Appl. Pharmacol.* 1965, **7**, 268.
7. Schumacher, H. et al *J. Pharm. Exp. Therap.* 1968, **160**, 189.
8. Stephens, T. D. *Teratology* 1988, **38**(3), 229-239.
9. Gaffield, W. et al *Stud. Nat. Prod. Chem.* 1990, **7**, 3-28.
10. Gunzler, V. *Drug Safety* 1992, **7**, 116-134.
11. Chen, T. L. et al *Drug Metab. Dispos.* 1989, **17**(4), 402-405.
12. Lisek, C. A. *Diss. Abstr. Int. B.* 1986, **47**(2), 613.
13. Gordon, G. B. et al *Proc. Nat. Acad. Sci. USA* 1981, **78**, 2545.
14. *Toxicol. Appl. Pharmacol.* 1972, **23**, 288.
15. Ashby, J. et al *Mutat. Res.* 1997, **396**(1,2), 45-64.
16. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
17. Akermann, H. et al *Gig. Sanit.* 1987, (2), 92-93 (Russ.) (*Chem. Abstr.* **106**, 151308q)

T100 thallium

TI

TI

Mol. Wt. 204.38

CAS Registry No. 7440-28-0

EINECS No. 231-138-1

RTECS No. XG 3425000

Uses In poisons for rats and other rodents. In alloys and semiconductors.

Occurrence In mineral ores such as crookesite, lorandite and hutchinsonite. Occurrence in Earth's crust 0.7 ppm.

Physical properties

M. Pt. 303.5°C B. Pt. 1457°C Specific gravity 11.85 Volatility v.p. 1 mmHg at 825°C

Occupational exposure

FR-VME 0.1 mg m⁻³

US-TWA 0.1 mg m⁻³

Supply classification very toxic

Risk phrases Very toxic by inhalation and if swallowed – Danger of cumulative effects (R26/28, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep away from food, drink and animal feeding stuffs – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S13, S28, S45)

Mammalian & avian toxicity

Acute data

TD_{Lo} oral man 5.7-14 mg kg⁻¹ (1,2).

TD_{Lo} oral child 10 mg kg⁻¹ (2).

Teratogenicity and reproductive effects

Skeletal deformities in offspring of laboratory animals exposed to thallium during early pregnancy have been reported (3).

Metabolism and toxicokinetics

Thallium salts injected intravenously into rabbits rapidly disappear from blood. Intravenous administration to the Japanese quail results in accumulation in brain, muscle and egg shells (4).

Intravenous rats (maximum tolerated dose), 31 to 38% was excreted in the faeces within 24 hr (5).

Other effects

Other adverse effects (human)

In humans and other species damage to nerves, nerve sheaths and muscle occurs (1).

Chronic poisoning in humans is accompanied by skin and nail atrophy, hair loss and central nervous system effects (2-3,6).

Acute poisoning in man is accompanied by nausea, vomiting, diarrhoea, colic, coma, convulsions and, if fatal, death within 10-12 days (7).

Any other adverse effects

The pharmacokinetics alter qualitatively with dose (8).

Changes in ATP concentration in tissue during the early period after thallium administration to mice may be closely related to changes in (Na⁺-K⁺)-ATPase activity (9).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (10).

Other comments

Occurs as an environmental pollutant (11,12).

Tissue distribution in humans and the effect of antidotes have been reviewed (13).

Sources and levels of thallium in the environment have been reviewed (12).

Neurotoxicity and reproductive toxicity reviewed (14,15).

Mutagenic, carcinogenic and teratogenic effects are reviewed (16).

Environmental health criteria for thallium reviewed (17).

References

1. *Archiv. Toxicol.* 1961, **19**, 65.
2. Browning, E. *Toxicity of Industrial Metals* 1961, Butterworths, London, UK.
3. Stevens, W. J. et al *Acta Clin. Belg.* 1976, **31**, 188.
4. Robinson, G. A. et al *Poult. Sci.* 1990, **69**(2), 300-306.
5. Gregus, Z. et al *Toxicol. Appl. Pharm.* 1986, **85**(1), 24-38.
6. Friberg, L. et al *Handbook on Toxicology of Metals* 1979, Elsevier, Amsterdam, Netherlands.
7. Paulson, G. et al *Arch. Intern. Med.* 1972, **129**, 100.
8. Morales-Aguilera, A. et al *Arch. Invest. Med.* 1990, **21**(3), 263-267.
9. Yoshida, M. et al *Bull. Environ. Contam. Toxicol.* 1997, **59**(2), 268-273.
10. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
11. Chapman, P. M. et al *Mar. Ecol. Prog. Ser.* 1987, **37**(1), 75-96.
12. Ewers, U. *Sci. Total Environ.* 1988, **71**(3), 285-292.
13. LeLoux, M. S. et al *J. Toxicol. Clin. Exp.* 1990, **10**(3), 147-156.
14. Cavanagh, J. B. *NATO ASI Ser., Ser. A* 1988, **100**, 177-202.
15. Formigli, L. et al *Heavy Metal Environ. Int. Conf.* 5th Conf. 1985, 215-218.
16. Leonard, A. et al *Mutat. Res.* 1997, **387**(1), 47-53.
17. *Environmental Health Criteria No.182: Thallium* 1996, WHO/IPCS Geneva, Switzerland

T101 thallium(I) acetate



$\text{C}_2\text{H}_3\text{O}_2\text{Tl}$

Mol. Wt. 263.43

CAS Registry No. 563-68-8

Synonyms thallium(I) methanoate; thallos acetate

EINECS No. 209-257-5

RTECS No. AJ 5425000

Uses In ore flotation. Previously used as a medicine for the treatment of ringworm and as an ingredient of depilatory creams.

Physical properties

M. Pt. 126-128°C **Specific gravity** 3.76 at 137°C

Solubility Organic solvents: chloroform, ethanol

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Tl) (inhalable dust fraction)

US-TWA 0.1 mg m⁻³ (as Tl)

UN No. 1707 **HAZCHEM Code** 2X **Conveyance classification** toxic substance

Supply classification very toxic

Risk phrases Very toxic by inhalation and if swallowed – Danger of cumulative effects (R26/28, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep away from food, drink and animal feeding stuffs – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S13, S28, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) Atlantic salmon 0.03 ppm as thallium (1).

LC₅₀ (96 hr) bluegill sunfish 170 ppm static bioassay at 23°C (2).

LC₅₀ (96 hr) inland silverside 31 ppm static bioassay at 23°C (2).

Invertebrate toxicity

LC₅₀ (96 hr) brown shrimp 10 ppm (1).

EC₅₀ (48 hr) *Daphnia magna* (Strauss test) <1 mg l⁻¹ (3).

Bioaccumulation

The bioconcentration factor in marine invertebrates was 150,000 and in freshwater and marine fish and plants 100,000. The bioconcentration factor in clams was 17-18, in mussels 11-12, and Atlantic salmon 27-1430 (4).

Environmental fate

Degradation studies

No evidence was found for the formation of volatile thallium compounds in the environment (4).

Natural thallium levels in plants are reported as 0.01-3800 ppm by weight; 0.5 ppm was the average value in most species (5).

Adsorption and retention

Thallium salts are strongly adsorbed by montmorillonite clays (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 35 mg kg⁻¹ (6).

LD₅₀ intraperitoneal rat 30 mg kg⁻¹ (6).

LD_{Lo} intravenous rabbit 26 mg kg⁻¹ (6).

Thallium salts are toxic when inhaled, ingested or absorbed through the skin. Symptoms of poisoning may appear within 12-24 hr of a single toxic dose and include severe abdominal pain, vomiting, diarrhoea, gastro-intestinal haemorrhage, tremors, delirium, convulsions, paralysis and coma leading to death in 1-2 days. The acute reaction may subside, to be followed in 10 days by the development of polyneuritis, psychosis, delirium encephalopathy, tachycardia, hypertension, skin eruptions and hepatorenal injury. Alopecia occurs within 15-20 days. Death may result from respiratory failure (7).

Sub-acute and sub-chronic data

In a 90-day feeding study in rats, 0.003% caused growth depression and depilation. Atrophy of hair follicles and sebaceous glands were observed in the skin. The kidney was the principal site of deposition in rats followed by bone, liver, lung, spleen and brain (8).

Newborn Wistar rats were given 16 mg kg⁻¹ thallium(I) acetate intraperitoneally on day 1 after birth in aqueous solution. At 8 days of age, sural nerves of thallium-treated rats showed a moderate reduction in the large and medium-sized fibres, and several of the myelin sheaths had initial degeneration along the course of the axon. Interstitial oedema was found in both neural and muscular tissues. Distinct features of focal necrosis as well as small haemorrhages were seen in peroneus muscle. At 50 days of age, the lesions were more diffuse. Large and small myelinated fibres were found to be sinuous, fragmented and scanty. Alterations in the large and medium sized axons were seen and the myelin sheaths were altered along the course of the axon. Additionally, muscle fibres had myopathic changes with abnormal central nucleoli, and the striated transverse fibres had disappeared in many areas of the sample. Several interstitial foci of muscular necrosis accompanied by phagocytosis and fibrosis were also present (9).

Teratogenicity and reproductive effects

In humans (and laboratory animals), following thallium poisoning, the testis had some of the highest thallium levels of any organ. The evidence suggests that reproductive systems are highly susceptible to thallium toxicity (5).

Metabolism and toxicokinetics

In humans, thallium was detected in urine, faeces and hair 5 months after a single exposure. Excretion takes place via the kidney, gut and salivary glands (5).

Excretory routes differ in importance for different species. Following (3 day) exposure to thallium by unspecified route(s), human faecal and urinary excretion was measured at 0.4% and 11.3%, respectively. In comparison, (2 day) rat faecal excretion was 9% and urinary 6%, and dog (36 day) urinary excretion was 60% (8).

Genotoxicity

Escherichia coli SOS chromotest negative (5).

Other effects

Any other adverse effects

In acute thallium poisoning, thallium accumulates in the grey matter of the brain (5).

In mouse myelinated cord-ganglia-muscle 10 µg ml⁻¹ caused enlarged mitochondria in the axons of peripheral nerve fibres within 2 hr (10).

Following inhalation of thallium and its salts, thallium was rapidly absorbed from mucous membranes of respiratory tract, mouth and lung. Distribution to the tissues was rapid via the blood; part of the thallium was absorbed into erythrocytes. Thallium crosses the blood/brain and placental barriers (11).

Other comments

UK legislation prohibits the use of thallium compounds in cosmetic products (7).

The toxicity of thallium and its salts is discussed in detail (8).

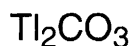
Thallium acetate as a hazardous material is reviewed (12).

Cases of human poisoning by thallium and its salts are reviewed (13-15).

References

1. Zitko, V. *The Science of the Total Environment* 1973, **4**, 185.
2. Dawson, G. W. et al *J. Haz. Mater.* 1975/77, **1**, 303-318.
3. Bringmann, G. et al *Z. Wasser Abwasser Forsch.* 1982, **15**(1), 1-6.
4. Callahan, M. A. et al *Water-Related Environmental Fate of 129 Priority Pollutants* 1979, **1**, EPA 440/4 79-029a.
5. Seiler, H. G. et al *Handbook on the Toxicity of Inorganic Compounds* 1988, 678, Marcel Dekker, New York, NY, USA.
6. Spector, W. S. (Ed.), *Handbook of Toxicology* 1956, **1**, 294-295, Saunders, Philadelphia, PA, USA.
7. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
8. *Patty's Industrial Hygiene and Toxicology* 3rd ed., 1981, **2**, Clayton, G. D. et al (Eds.), John Wiley, New York, NY, USA.
9. Barroso-Moguel, R. et al *J. Appl. Toxicol.* 1996, **16**(5), 385-389.
10. Spencer, P. S. et al *J. Cell Biol.* 1973, **58**, 79.
11. Venugopal, B. et al *Metal Toxicity in Mammals* 1978, (2), Plenum Press, New York, NY, USA.
12. *Dangerous Prop. Ind. Mater. Rep.* 1987, **7**(2), 92-94.
13. Conley, B. E. *J. Am. Med. Assoc.* 1957, **165**, 1566.
14. Munch, J. C. *J. Am. Med. Assoc.* 1934, **102**, 1929.
15. Poliakova, M. M. *Gig. Tr. Prof. Zabol.* 1977, **2**, 14

T102 thallium(I) carbonate



CO₃Ti₂

Mol. Wt. 468.78

CAS Registry No. 6533-73-9

Synonyms thalious carbonate; thallium(1+) carbonate; carbonic acid, dithallium(1+) salt; dithallium carbonate

EINECS No. 229-434-0

RTECS No. XG 4000000

Uses In manufacture of imitation diamonds.

Physical properties

M. Pt. 272°C Specific gravity 7.11

Solubility Water: soluble in 24 parts of water

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as TI) (inhalable dust fraction)

UK-LTEL 0.1 mg m⁻³ (as TI)

US-TWA 0.1 mg m⁻³ (as TI)

UN No. 1707 HAZCHEM Code 2X Conveyance classification toxic substance

Supply classification very toxic

Risk phrases Very toxic by inhalation and if swallowed – Danger of cumulative effects (R26/28, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep away from food, drink and animal feeding stuffs – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S13, S28, S45)

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 21, 23 mg kg⁻¹, respectively (1).

LD₅₀ dermal rat 117 mg kg⁻¹ (2).

LD₅₀ subcutaneous mouse 27 mg kg⁻¹ (3).

Teratogenicity and reproductive effects

Oral ♂ mice (6 month) 1 and 10 µg l⁻¹ in drinking water. 1 µg l⁻¹ decreased sperm motility and 10 µg l⁻¹ lowered the fertility of spermatozoa (4).

Genotoxicity

Induced single-strand DNA breaks in cultured rat and mouse embryo cells and dominant lethal mutations in rats after oral administration (5).

Induced sister chromatid exchanges and chromosomal aberrations in Chinese hamster ovary cells (6).

Legislation

Reportable under US Federal Comprehensive Environmental Response, Compensation and Liability Act (7).

Land disposal prohibited under US Federal Resource Conservation and Recovery Act (8).

References

1. Hyg. Sanit. 1964, 29, 26.
2. Gig. Tr. Prof. Zabol. 1980, 24(4), 54.
3. Toksikol. Nov. Prom. Khim. Veschestv. 1961, 2, 94.
4. Wei, Q. Zhonghua Yufangyixue Zazhi 1987, 21(3), 141-143 (Ch.) (Chem. Abstr. 107, 192558k).
5. Zasukhina, G. D. et al Mutat. Res. 1983, 124, 163-173.
6. Zhang, D. Huanjing Kexue 1988, 9(2), 29-32 (Ch.) (Chem. Abstr. 109, 33382y).
7. Fed. Regist. 1989, 54(155), 33426-33484.
8. Fed. Regist. 1991, 56(21), 3864-3928

T103 thallium(I) chloride

TICI

CITI

Mol. Wt. 239.84

CAS Registry No. 7791-12-0

Synonyms thallos chloride; thallium monochloride

EINECS No. 232-241-4

RTECS No. XG 4200000

Uses Catalyst. Thallos chloride (^{207}Tl) is used intravenously to investigate coronary heart disease, infarction and for post-surgical assessment of bypass patency.

Physical properties

M. Pt. 430°C B. Pt. 720°C Specific gravity 7.00 Volatility v.p. 10 mmHg at 517°C

Solubility Water: 3.3 g l⁻¹ at 20°C

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Tl) (inhalable dust fraction)

UK-LTEL 0.1 mg m⁻³ (as Tl)

US-TWA 0.1 mg m⁻³ (as Tl)

UN No. 1707 HAZCHEM Code 2X Conveyance classification toxic substance

Supply classification very toxic

Risk phrases Very toxic by inhalation and if swallowed – Danger of cumulative effects (R26/28, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep away from food, drink and animal feeding stuffs – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S13, S28, S45)

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 24 mg kg⁻¹ (1).

LD₅₀ intraperitoneal mouse 28 mg kg⁻¹ (2).

Teratogenicity and reproductive effects

A minor increase in post-implantation loss reported in mice after oral administration of 6 mg kg⁻¹ on days 6-15 of pregnancy (3).

Genotoxicity

Salmonella typhimurium (strains and metabolic activation unspecified) negative (40).

Escherichia coli PQ37 SOS chromotest with or without metabolic activation negative (4).

Enhanced transformation of Syrian hamster embryo cells by a Simian adenovirus, SA7, *in vitro* (5).

Legislation

Reportable under US Federal Comprehensive Environmental Response, Compensation and Liability Act (6).

Land disposal prohibited under US Federal Resource Conservation and Recovery Act (7).

References

1. Hyg. Sanit. 1964, 29, 26.
2. C. R. Hebd. Seances Acad. Sci. 1963, 256, 1043.
3. Roll, R. et al Teratology 1981, 24(2), 41A-47A.
4. von der Hude, W. et al Mutat. Res. 1988, 203(2), 81-94.

5. Casto, B. C. et al *Cancer Res.* 1979, **39**, 193-198.
6. *Fed. Regist.* 1989, **54**(155), 33426-33484.
7. *Fed. Regist.* 1991, **56**(21), 3864-3928

T104 thallium hydrogen sulfate



HO₄STI

Mol. Wt. 301.45

CAS Registry No. 10031-59-1

Synonyms sulfuric acid, thallium salt

RTECS No. XG 6600000

Physical properties

M. Pt. 632°C B. Pt. decomp. Specific gravity 6.77

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as TI) (inhalable fraction of aerosol)

UK-LTEL 0.1 mg m⁻³ (as TI)

US-TWA 0.1 mg m⁻³ (as TI)

UN No. 1707 HAZCHEM Code 2X Conveyance classification toxic substance

Supply classification very toxic

Risk phrases Very toxic by inhalation and if swallowed – Danger of cumulative effects (R26/28, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep away from food, drink and animal feeding stuffs – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S13, S28, S45)

Mammalian & avian toxicity

Acute data

LD_{Lo} oral human 7 mg kg⁻¹ (1).

LD₅₀ oral mouse, rat 15, 16 mg kg⁻¹, respectively (2,3).

LD₅₀ intravenous rat 12 mg kg⁻¹ (4).

Teratogenicity and reproductive effects

Significantly reduced foetal body weight, hydronephrosis and non-ossification of vertebrae reported, but no increase in resorptions, in rats administered intraperitoneally at 2.5 mg kg⁻¹ on days 8, 9 and 10 or 2.5-10 mg kg⁻¹ on days 12, 13 and 14 of pregnancy (5).

Other comments

Environmental health criteria for thallium reviewed (6).

References

1. *Pesticide Chemicals Official Compendium* 1966, 1126, Assoc. Am. Pest. Control Officials Inc., Topeka, KS, USA.
2. *Yakkyoku* 1977, **28**, 329.
3. *J. Am. Med. Assoc.* 1945, **129**, 927.
4. *Toxicol. Appl. Pharmacol.* 1967, **10**, 199.
5. Gibson, J. E. et al *Toxicol. Appl. Pharmacol.* 1970, **16**, 120-132.
6. *Environmental Health Criteria No.182: Thallium* 1996, WHO/IPCS, Geneva, Switzerland

T105 thallium(I) malonate



$\text{C}_3\text{H}_2\text{O}_4\text{Tl}_2$

Mol. Wt. 510.81

CAS Registry No. 2757-18-8

Synonyms thallos malonate; formomalenic thallium; malonic acid, thallium salt; propanedioic acid, dithallium salt

EINECS No. 220-414-7

RTECS No. OO 1770000

Occupational exposure

UK-LTEL 0.1 mg m⁻³ (as Tl)

US-TWA 0.1 mg m⁻³ (as Tl)

UN No. 1707 HAZCHEM Code 2X Conveyance classification toxic substance

Supply classification very toxic

Risk phrases Very toxic by inhalation and if swallowed – Danger of cumulative effects (R26/28, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep away from food, drink and animal feeding stuffs – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S13, S28, S45)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 18,000 µg kg⁻¹ (1).

LD₅₀ dermal rat 57,700 µg kg⁻¹ (1).

References

1. *Gig. Tr. Prof. Zabol.* 1976, 20(8), 35

T106 thallium(I) nitrate



NO_3Tl

Mol. Wt. 266.39

CAS Registry No. 10102-45-1

Synonyms nitric acid, thallium(I) salt; thallium mononitrate; thallos nitrate

EINECS No. 233-273-1

RTECS No. XG 5950000

Uses Chemical reagent. Used in green marine flares.

Physical properties

M. Pt. 206°C B. Pt. 450°C (decomp.) Specific gravity 5.55

Solubility Water: 100 g l⁻¹ in cold water; 3300 g l⁻¹ at 100°C

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Tl) (inhalable dust fraction)

FR-VME 0.1 mg m⁻³

UK-LTEL 0.1 mg m⁻³ (as TI)

US-TWA 0.1 mg m⁻³ (as TI)

UN No. 2727 HAZCHEM Code 2W Conveyance classification toxic substance, fire intensifying hazard

Supply classification very toxic

Risk phrases Very toxic by inhalation and if swallowed – Danger of cumulative effects (R26/28, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep away from food, drink and animal feeding stuffs – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S13, S28, S45)

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 33 mg kg⁻¹ (1).

LD₅₀ oral dog 45 mg kg⁻¹ (2).

LD₅₀ intraperitoneal rat 21 µg kg⁻¹ (3).

LD₅₀ intravenous rabbit 14 mg kg⁻¹ (4).

TD_{Lo} oral man 73 mg kg⁻¹ (5).

Metabolism and toxicokinetics

Absorption is rapid and sometimes complete following oral, subcutaneous, intraperitoneal, intramuscular, and intravenous administration to rats (6).

It is well distributed within tissues and can cross the placental barrier (6,7).

It is rapidly removed from plasma and ~6% of dose is excreted in urine within 24 hr, dropping to 0.5% by the 10th day after dosing (6,8).

In both animals and humans, excretion is by urine and faeces with quantities being detectable in other secretions including breast milk (7).

Genotoxicity

Bacillus subtilis rec⁺rec⁻ DNA damage positive (9).

Other effects

Other adverse effects (human)

Chronic poisoning in humans is accompanied by skin and nail atrophy, hair loss, neurotoxic and central nervous system effects (10,11).

Acute toxicity in humans is accompanied by nausea, vomiting, colic, coma, convulsions and, if fatal, death within 10-12 days. Cardiovascular and neurotoxic effects can also be observed (10,11).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Nitrates: guide level 25 mg l⁻¹, maximum admissible concentration 50 mg l⁻¹ (12).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (13).

Toxicology reviewed (14).

References

1. *J. Fac. Agric. Tottoro Univ.* 1969, **5**, 15.
2. Spector, W. S. (Ed.) *Handbook of Toxicology* 1956, **1**, Saunders, Philadelphia, PA, USA.
3. *Arch. Int. Pharmacodyn. Therap.* 1969, **182**, 425.
4. *Environ. Qual. Safety Suppl.* 1935, **4**, 1406.
5. *Forensic Medical Examination* 1975, **18**(4), 37.

6. Lie, R. et al *Health Phys.* 1960, **2**, 334-340.
7. Heyroth, F. F. *U.S. Pub. Hlth. Serv. Pub. Hlth. Rep. Suppl.* 197, 1947.
8. Rauws, A. G. *Arch. Pharmacol.* 1974, **284**, 295-306.
9. Kanematsu, N. et al *Mutat. Res.* 1980, **77**, 109-116.
10. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
11. Friberg, L. et al *Handbook on Toxicology of Metals* 1979, Elsevier, Amsterdam, Netherlands.
12. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
13. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
14. *Dangerous Prop. Ind. Mater. Rep.* 1988, **8**(4), 13-22

T107 thallium(III) oxide



O_3Tl_2

Mol. Wt. 456.76

CAS Registry No. 1314-32-5

Synonyms thallium(III) oxide; thallium(3+) oxide; dithallium trioxide; thallium sesquioxide; thallium peroxide

EINECS No. 215-229-3

RTECS No. XG 2975000

Uses Chemical intermediate.

Physical properties

M. Pt. 717°C B. Pt. 875°C Specific gravity 9.65

Occupational exposure

UN No. 1707 HAZCHEM Code 2X Conveyance classification toxic substance

Supply classification very toxic

Risk phrases Very toxic by inhalation and if swallowed – Danger of cumulative effects (R26/28, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep away from food, drink and animal feeding stuffs – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S13, S28, S45)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 44 mg kg⁻¹ (1).

LD_{Lo} oral rabbit 34 mg kg⁻¹ (1).

LD_{Lo} oral dog 34 mg kg⁻¹ (1).

LD_{Lo} intraperitoneal rat 103 mg kg⁻¹ (1).

LD_{Lo} intraperitoneal rabbit 67 mg kg⁻¹ (1).

LD_{Lo} intravenous rabbit 44 mg kg⁻¹ (1).

LD_{Lo} intraperitoneal guinea pig 34 mg kg⁻¹ (2).

Other comments

The toxicity of thallium compounds has been reviewed (2,3).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (4).

References

1. *Am. Ind. Hyg. Assoc. J.* 1960, **21**, 399.
2. Venugopal, B. et al *Metal Toxicity in Mammals* 2 1978, Plenum Press, New York, NY, USA.
3. Friberg, L. et al *Handbook on Toxicology of Metals* 1979, Elsevier, Amsterdam, Netherlands.
4. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T108 thallium(I) sulfate



O₄STl₂

Mol. Wt. 504.83

CAS Registry No. 7446-18-6

Synonyms sulfuric acid, dithallium(1+) salt; sulfuric acid, thallium(1+) salt; dithallium sulfate; thallosulfate; ecothal

EINECS No. 231-201-3

RTECS No. XG 6800000

Uses Rat poison and ant bait. Analytical reagent.

Physical properties

M. Pt. 632°C **Specific gravity** 6.77

Solubility Water: 27 g l⁻¹ at 20°C

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Tl) (inhalable dust fraction)

FR-VME 0.1 mg m⁻³

UK-LTEL 0.1 mg m⁻³ (as Tl)

US-TWA 0.1 mg m⁻³ (as Tl)

UN No. 1707 **HAZCHEM Code** 2X **Conveyance classification** toxic substance

Supply classification very toxic

Risk phrases Very toxic if swallowed – Irritating to the skin – Toxic: danger of serious damage to health by prolonged exposure if swallowed (R28, R38, R48/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep away from food, drink and animal feeding stuffs – Wear suitable protective clothing and gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S13, S36/37, S45)

Mammalian & avian toxicity

Acute data

LD₅₀ oral starling 34.6-56.6 mg kg⁻¹ (1).

LD₅₀ oral rat 25 mg kg⁻¹ (2).

LD₅₀ oral mouse 29 mg kg⁻¹ (3).

LD₅₀ subcutaneous mouse 26 mg kg⁻¹ (4).

LD_{Lo} oral man 7-3000 µg kg⁻¹ (5,6).

Acute effects seen in mammals, including man: damage to the cardiovascular, gastro-intestinal, central and peripheral nervous systems (5-8).

Reduced sensitivity to cardiac vascular stimuli is frequently seen (7).

Accompanying changes in biochemical parameters such as increased serum γ-GTP and creatinine are also observed (8,9).

Sub-acute and sub-chronic data

Rats orally administered with $0.05 \times \text{LD}_{50}$ dose daily for 3 months showed an increase in serum GPT, increased bilirubin production and increases in blood urea and serum creatinine (9).

Teratogenicity and reproductive effects

Female rats receiving 0.001% thallium sulfate during pregnancy bore offspring with hair development that was retarded for the first 50 days of life. Hypertensive and hypotensive responses were impaired for up to 60 days (10).

Rats receiving 2.5-10 mg kg⁻¹ on days 8-10 or 12-14 of pregnancy showed lethargy, hair loss and diarrhoea, while offspring had a low foetal weight, some hydronephrosis and missing vertebral bodies (11).

Achondroplasia is seen in chick embryos exposed to the compound (12,13).

Metabolism and toxicokinetics

The salt is rapidly absorbed following ingestion, inhalation or skin contact. It is distributed to all tissues, but penetrates the brain more slowly than other tissues (14,15).

It can cross the placental barrier to produce tissue concentrations 1/15 of that in maternal plasma (15).

It is detected in urine within 1 hr of oral administration to rats and has a biological $t_{1/2}$ 4 days (15).

In hamsters, 47.4 % is eliminated within 7 days of an oral dose of 10 mg TI l⁻¹, with both urinary and faecal elimination being seen (16).

Other effects

Other adverse effects (human)

Chronic poisoning in humans is accompanied by skin and nail atrophy, hair loss, neurotoxic and central nervous system effects (8,17).

Peripheral blood lymphocytes from a patient who had ingested 200 mg of thallium sulfate were examined in order to evaluate the ability of the compound to produce cytogenetic damage *in vivo* in humans. Neither the yield of structural chromosome aberrations nor sister chromatid exchanges were significantly modified. The drastic increase in binucleated cells with micronuclei indicated that thallium sulfate has, in common with many metallic compounds, the ability to interfere with chromosome distribution (18).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Sulfates: guide level 25 mg l⁻¹, maximum admissible concentration 250 mg l⁻¹ (19).

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (20).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (21).

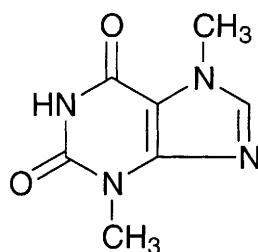
Cytotoxicity has been assessed (22).

References

1. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
2. Schafer, E. W. *Toxicol. Appl. Pharmacol.* 1972, **21**, 315.
3. *J. Fac. Agric. Tottoro Univ.* 1969, **5**, 15.
4. *Medycine Pracy. Indust. Med.* 1979, **30**, 257.
5. *Am. J. Cardiol.* 1943, **13**, 422.
6. *Clin. Toxicol. (New York)* 1980, **1**, 133.
7. Rossi, F. et al *Curr. Ther. Res.* 1987, **42**(5), 778-789.
8. Friberg, L. et al *Handbook on Toxicology of Metals* 1979, Elsevier, Amsterdam, Netherlands.
9. El-Garawang, et al *Egypt. J. Pharm. Sci.* 1990, **31**(1-4), 331-336.
10. Matera, M. G. et al *Rend. Atti Accad. Sci. Med. Chir.* 1986, **140**, 177-202 (Ital.) (*Chem. Abstr.* **107**, 213185d).
11. Gibson, J. E. *Toxicol. Appl. Pharmacol.* 1970, **16**, 120-132.
12. Hall, B. K. et al *Can. J. Zool.* 1972, **50**(12), 1527-1536.
13. Kanofsky, D. A. et al *Proc. Soc. Exp. Biol. Med.* 1950, **73**, 255-259.

14. Lund, A. *Acta Pharmacol. Toxicol.* 1956, **12**, 251-268.
15. Rauws, A. G. *Arch. Pharmacol.* 1974, **284**, 295-306.
16. Aoyama, H. *Sei. Marianna Ika Daigaku Zasshi* 1988, **16**(3), 325-334.
17. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
18. Hantson, P. et al *J. Toxicol. Environ. Health* 1997, **50**(2), 97-100.
19. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
20. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
21. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
22. Hulme, L. et al *Mol. Toxicol.* 1987, **1**(4), 589-596

T109 theobromine



$C_7H_8N_4O_2$

Mol. Wt. 180.17

CAS Registry No. 83-67-0

Synonyms 3,7-dihydro-3,7-dimethyl-1H-purine-2,6-dione; 3,7-dimethylxanthine; diurobromine; Thesal

EINECS No. 201-494-2

RTECS No. XH 2275000

Uses Diuretic, bronchodilator, cardiotonic.

Occurrence Principal alkaloid in cacao beans, also present in tea.

Physical properties

M. Pt. 357°C **B. Pt.** 290-295°C (sublimes).

Solubility Water: 0.5 g l⁻¹

Mammalian & avian toxicity

Acute data

LD₅₀ oral dog, mouse, rat 300, 837, 1265 mg kg⁻¹, respectively (1,2).

LD₅₀ subcutaneous mouse 530 mg kg⁻¹ (3).

LD_{Lo} subcutaneous rabbit 1 g kg⁻¹ (4).

Sub-acute and sub-chronic data

Marked changes in thymus and testes reported in rabbits fed up to 1.5% for 20 or 120 days (5).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (6).

Teratogenicity and reproductive effects

Reduced litter size, live pups litter⁻¹ and pup body-weight reported in mice administered 0.25 and 0.5% in feed to ♂ and ♀ (7).

Retarded spermatogenesis in rats given three oral daily doses of 500 mg kg⁻¹ (8).

Metabolism and toxicokinetics

48 hr after ingesting 1 g, human volunteers excreted in urine theobromine (12.05%), 3-methylxanthine (19.85%), 7-methylxanthine (28.05%) and 7-methyluric acid. Demethylation in humans can occur at the 1, 3 and 7 positions, 1 being the most, and 3 the least, stable. Demethylation does not appear to proceed beyond the monomethylxanthine stage as there is no accumulation of xanthine in urine or increase in uric acid excretion (9). Metabolised to 6-amino-5-(*N*-methylformylamino)-1-methyluracil, 3,7-dimethyluric acid, 3-methylxanthine and 7-methylxanthine when incubated with rat hepatic microsomes (10).

Genotoxicity

Salmonella typhimurium TA100 with and without metabolic activation negative (11).

Escherichia coli (metabolic activation unspecified) positive (9).

Induced chromosome breaks in HeLa cells and cultured human lymphocytes (9).

High concentrations are antimitotic and cytostatic to human peripheral blood lymphocytes, but did not cause chromosomal damage (12).

Did not induce chromosomal aberrations in Chinese hamster ovary cells with or without metabolic activation, or transformation in Bab/C-3T3 cells (11).

Mouse lymphoma L5178Y cell forward mutation assay with and without metabolic activation negative (11).

Induced sister chromatid exchanges in human lymphocytes and Chinese hamster ovary cells without metabolic activation (11).

Other effects

Other adverse effects (human)

Central nervous system and cardiac muscle stimulant, diuretic, smooth muscle relaxant (11).

Large doses can cause nausea and vomiting (13).

Other comments

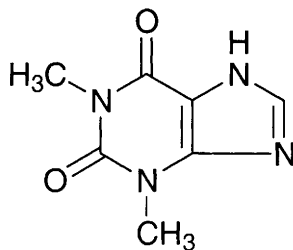
Pharmacokinetics reviewed (14,15).

Human toxicity reviewed (16).

References

1. *Toxicol. Appl. Pharmacol.* 1980, **53**, 481.
2. *Gig. Tr. Prof. Zabol.* 1982, **26**(3), 59.
3. *Arzneim.-Forsch.* 1956, **6**, 601.
4. *Abdernalden's Handbuch der Biologischen Arbeitsmethoden* 1935, **4**, 1289, Leipzig, Germany.
5. Soffietti, M. G. et al *J. Comp. Pathol.* 1989, **100**(1), 47-58.
6. *IARC Monograph.* 1987, **Suppl.** 7.
7. Choudhury, H. et al *Toxicologist* 1984, **4**, 191.
8. Ettlin, R. A. et al *Arch. Toxicol. Suppl.* 1986, **9**(Toxic Interfaces Neurones, Smoke Genes), 441-446.
9. Timson, J. *Mutat. Res.* 1975, **32**, 169-172.
10. Lelo, A. et al *J. Chromatogr.* 1988, **430**(1), 203-206.
11. Brusick, D. et al *Mutat. Res.* 1986, **169**, 105-114.
12. Timson, J. *Mutat. Res.* 1972, **15**, 197-201.
13. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
14. Leolo, A. et al *Br. J. Clin. Pharmacol.* 1986, **22**, 177.
15. Tarka, S. M. et al *Clin. Pharmacol. Ther.* 1983, **34**, 546-555.
16. Stavric, B. *Food Chem. Toxicol.* 1988, **26**(8), 725-733

T110 theophylline



C₇H₈N₄O₂

Mol. Wt. 180.17

CAS Registry No. 58-55-9

Synonyms 3,7-dihydro-1,3-dimethyl-1*H*-purine-2,6-dione; 1,3-dimethylxanthine

EINECS No. 200-385-7

RTECS No. XH 3850000

Uses Bronchodilator used in emergency and chronic treatment of asthma.

Occurrence Present in small amounts in tea.

Physical properties

M. Pt. 270-274°C

Solubility Water: 8.33 g l⁻¹. Organic solvents: chloroform, ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 244, 252 mg kg⁻¹, respectively (1).

LD_{Lo} oral dog, cat 290, 800 mg kg⁻¹, respectively (2).

LD₅₀ intraperitoneal mouse, rat 70, 188 mg kg⁻¹, respectively (3,4).

LD₅₀ subcutaneous rat, mouse 75, 180 mg kg⁻¹, respectively (5,6).

LD₅₀ intravenous mouse 136 mg kg⁻¹ (7).

TD_{Lo} oral woman, child, man 5, 10, 129 mg kg⁻¹, respectively (8-10).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (11).

Teratogenicity and reproductive effects

Reduced testicular weight reported in rats and mice administered 150 and 300 mg kg⁻¹ day⁻¹, respectively, for 13 wk; abnormal sperm reported in rats given up to 0.4% in feed. In continuous breeding reproductive assays in mice fed up to 530 mg kg⁻¹ day⁻¹ for 14 wk, there was a dose-dependent decrease in live pups litter⁻¹, litters pair⁻¹, live pup weight and percentage of pups born alive (12).

Decreased number of live foetuses litter⁻¹ and foetal weight, but no malformations reported in rats and mice fed up to 259 and 396 mg kg⁻¹ day⁻¹, respectively on day 6-15 of pregnancy (13).

Metabolism and toxicokinetics

Readily and completely absorbed via the gut in humans; in the 48 hr following ingestion of 1 g, urinary metabolites were 3-methylxanthine (13.3%), theophylline (9.9%), 1-methyluric acid (18.6%), and 1,3-diethyluric acid (35%). The major metabolic pathway is oxidation without demethylation (14).

Rate of absorption from the gut is decreased by food. Peak serum concentrations occur 1-2 hr after ingestion, or 4-12 hr if a sustained-release formulation is used. 60% is bound to plasma proteins (40% in neonates or adults with liver disease). Hepatic metabolism varies considerably between individuals, and is also affected by diet, drug interactions, smoking and disease. Serum t_{1/2} in an asthmatic, but otherwise healthy, non-smoking adult is 7-9 hr. Serum t_{1/2} in smokers and children is 4-5 and 3-4 hr, respectively. It crosses the placenta and is also secreted in milk (15).

Absorbed through the skin of mice, mean plasma concentration of 0.1 µg ml⁻¹ reported after topical administration of 0.1 mg (16).

85% of an intravenous dose of 8.2 mg kg⁻¹ was eliminated in urine of dogs within 24 hr; metabolites included 3-methylxanthine and 1,3-dimethyluric acid (17).

17.55% of an intravenous dose of 6 mg kg⁻¹ to humans was excreted unchanged in urine; the remainder was metabolised to 3-methylxanthine (11.62%), 1-methyluric acid (17.64%) and 1,3-dimethyluric acid (35.14%) (18).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535 with and without metabolic activation negative (19).

Escherichia coli (metabolic activation unspecified) positive (14).

Induced chromosome breaks in HeLa cells and human lymphocytes *in vitro* (14).

High concentrations are antimitotic and cytostatic in cultured human peripheral blood lymphocytes, but did not cause chromosome damage (20).

Weak inhibitor of DNA synthesis in human EUE cells *in vitro* and very weakly mutagenic in Chinese hamster V79 cells without metabolic activation (21).

Other effects

Other adverse effects (human)

Adverse effects commonly affect the gastro-intestinal tract (nausea, vomiting, abdominal pain, gastro-intestinal bleeding) and the central nervous system (insomnia, anxiety, headache and palpitation). Severe overdose causes maniacal behaviour, diuresis, repeated vomiting with extreme thirst, tremor, delirium, hyperthermia, tachycardia, tachypnoea, electrolyte disturbances, convulsions and death. Severe toxicity may not be preceded by milder symptoms. Hypotension may follow intravenous injection and sudden deaths have been reported. Proctitis may follow repeated administration of suppositories (15).

Other comments

Use in asthma (22) and pharmacology (23) reviewed.

Bioavailability and pharmacokinetics reviewed (24,25).

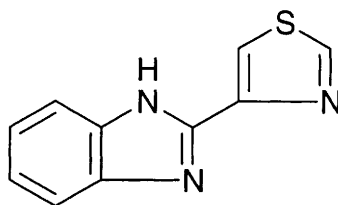
Human toxicity reviewed (26).

References

1. *Gig. Tr. Prof. Zabol.* 1982, **26**(3), 59.
2. *Deutsch. Arch. Klin. Med.* 1904, **80**, 510.
3. *Br. J. Pharmacol.* 1981, **73**, 887.
4. *Pediatr. Res.* 1977, **11**, 783.
5. *Fundam. Appl. Toxicol.* 1981, **1**, 443.
6. *Therapie* 1949, **4**, 28.
7. *Pharm. Acta Helv.* 1973, **48**, 133.
8. *Southwest. Med. J.* 1985, **78**, 1000.
9. *Br. Med. J.* 1984, **288**, 1497.
10. *Ann. Intern. Med.* 1986, **104**, 284.
11. *IARC Monograph.* 1987, **Suppl. 7**.
12. Morissey, R. E. et al *Fundam. Appl. Toxicol.* 1988, **10**(3), 525-536.
13. Lindstrom, P. et al *Fundam. Appl. Toxicol.* 1990, **14**(1), 167-178.
14. Timson, J. *Mutat. Res.* 1975, **32**, 169-178.
15. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
16. Bailey, D. N. J. *Toxicol. Cutaneous Ocul. Toxicol.* 1987, **6**(1), 29-32.
17. Kuze, T. et al *Nippon Yakurigaku Zasshi* 1988, **91**(5), 325-334 (Japan.) (*Chem. Abstr.* **109**, 22m).
18. Choi, H. R. et al *Chungang Uidaechi* 1989, **14**(2), 175-185 (Korean) (*Chem. Abstr.* **111**, 166741c).
19. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-157.
20. Timson, J. *Mutat. Res.* 1972, **15**, 197-201.
21. Slamenova, D. et al *Neoplasma* 1986, **33**(6), 699-706.

22. *Am. J. Med.* 1985, **79**(6A), 1-78.
23. *J. Allerg. Clin. Immunol.* 1986, **78**, 669-824.
24. Vural, I. et al *FABAD J. Pharm. Sci.* 1989, **14**(3), 190-200 (Turk.) (*Chem. Abstr.* **112**, 25421g).
25. Jerne, J. W. *Lung Biol. Health Dis.* 1987, **31** (Drug Ther. Asthma), 297-334.
26. Stavric, B. *Food Chem. Toxicol.* 1988, **26**(6), 541-565

T111 thiabendazole



C₁₀H₇N₃S

Mol. Wt. 201.25

CAS Registry No. 148-79-8

Synonyms 2-(thiazol-4-yl)benzimidazole; 4-(2-benzimidazolyl)thiazole

EINECS No. 205-725-8

RTECS No. DE 0700000

Uses Fungicide, anthelmintic.

Physical properties

M. Pt. 304-305°C **B. Pt.** sublimes above 310°C

Solubility Water: 10 g l⁻¹ at pH 2 and <0.05 g l⁻¹ at pH 5-12 (25°C). Organic solvents: dimethylformamide, dimethyl sulfoxide

Ecotoxicity

Fish toxicity

Low toxicity to fish (1).

Invertebrate toxicity

LC₅₀ (96 hr) *Nitocra spinipes* 24 mg l⁻¹ (2).

EC₅₀ (5 min) *Photobacterium phosphoreum* 3418 ppm Microtox test (3).

Not toxic to bees (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat, chicken 1395, 3100, 4000 mg kg⁻¹, respectively (5-7).

Carcinogenicity and chronic effects

No-effect level in 2-yr feeding trials in rats 40 mg kg⁻¹ day⁻¹ (1).

Teratogenicity and reproductive effects

Significant and dose-dependent increases in resorptions and decreases in number of live foetuses and foetal weight reported in rats after oral administration of 296-1000 mg kg⁻¹ day⁻¹ on days 8-15 of pregnancy; deformed limbs and tails occurred in groups treated on days 10, 11 or 12 (8).

Metabolism and toxicokinetics

Hydroxylated at the 5-position in mammals; 87% of oral dose eliminated in urine within 24 hr (9).
5-hydroxylated thiabendazole, its glucuronide and sulfate were identified as urinary and faecal metabolites in pregnant mice. Very small amounts of *N*-methylthiabendazole were also identified in urine. ~97% of the dose was excreted in urine and faeces within 7 days (10).

Genotoxicity

Salmonella typhimurium TA98 with metabolic activation positive, TA100 with or without metabolic activation negative, TA98 without metabolic activation negative (11).

Induced mitotic malsegregation of chromosome VII in *Saccharomyces cerevisiae* D61.M (12,13).

Saccharomyces cerevisiae D5 and XV185-14c negative (14).

In vitro micronucleus test positive (15).

Oral ♂ CD-1 mice 200 mg kg⁻¹ induced DNA damage in the stomach, liver, kidney, bladder and lung, as measured by a modified Comet assay at 3, 8 and 24 hr after administration (16).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (17).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (18).

WHO Toxicity Class Table 5 (19).

EPA Toxicity Class III (formulation) (4).

ADI (JMPR) 0.1 mg kg⁻¹ (4).

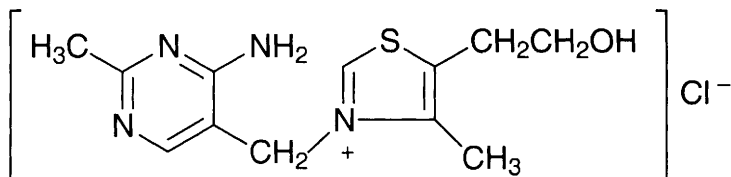
Other comments

Pharmacology reviewed (20).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. Linden, E. et al *Chemosphere* 1979, **11/12**, 843-851.
3. Kaiser, K. L. E. *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
5. *Farmakol. Toksikol. (Moscow)* 1971, **34**, 483.
6. *Toxicol. Appl. Pharmacol.* 1965, **7**, 53.
7. *Vet. Med. Nauk* 1982, **19**(3), 99.
8. Ogata, A. et al *Kenkyo Nenpo-Tokyo-toritsu Eisei Kenkyusho* 1986, **37** 421-425 (Japan.) (*Chem. Abstr.* **106**, 131305h).
9. Fujitaui, T. et al *Food Chem. Toxicol.* 1991, **29**(4), 265-274.
10. Tsuchiya, T. et al *Chem. Pharm. Bull.* 1987, **35**(7), 2985-2993.
11. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-157.
12. Albertini, S. *Mutagenesis* 1990, **5**(5), 453-459.
13. Antoccia, A. et al *Mutagenesis* 1991, **6**(4), 319-324.
14. Hennig, U. G. G. et al *Mutat. Res.* 1987, **187**(2), 79-89.
15. Mudry de Pargament, M. D. et al *Mutat. Res.* 1987, **188**(1), 1-6.
16. Sasaki, Yu. F. et al *Mutat. Res.* 1997, **395**(2,3), 189-198.
17. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
18. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
19. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
20. Kapoor, V. K. *Drug. Subst.* 1987, **16**, 611-639

T112 thiamine



C₁₂H₁₇N₄OSCl

Mol. Wt. 300.81

CAS Registry No. 59-43-8

Synonyms 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methylthiazolium chloride; thiamine chloride; thiamin; vitamin B₁

EINECS No. 200-425-3

RTECS No. XI 6550000

Physical properties

M. Pt. 260°C (decomp.) (HCl)

Solubility Water: 28.6 g l⁻¹. Organic solvents: slightly soluble in acetone and chloroform

Mammalian & avian toxicity

Acute data

LD₅₀ subcutaneous mouse, rat 301, 560 mg kg⁻¹, respectively (1,2).

LD₅₀ intravenous mouse, rat 83, 118 mg kg⁻¹, respectively (2).

Other comments

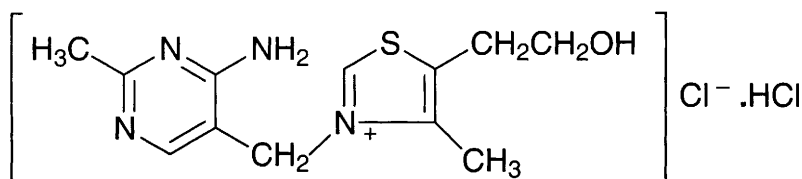
Thiamine treatment of humans with acquired thiamine deficiency reviewed (3).

Metabolism by humans with alcohol addiction reviewed (4).

References

1. *J. Pharmacol. Exp. Ther.* 1975, **119**, 444.
2. *Arzneim.-Forsch.* 1959, **9**, 1.
3. De Meirleir, L. J. *Voeding* 1990, **51**(12), 304-306.
4. Halsted, C. H. et al *Pharmacol. Ther.* 1987, **34**(3), 453-464

T113 thiamine hydrochloride



$C_{12}H_{18}N_4OSCl_2$

Mol. Wt. 337.27

CAS Registry No. 67-03-8

Synonyms thiamine chloride hydrochloride; thiamine dichloride; thiaminium chloride hydrochloride; vitamin B₁

EINECS No. 200-641-8

RTECS No. XI 7350000

Uses Enzyme co-factor vitamin, nutritional vitamin.

Occurrence In plants and animal tissues, especially rice husk, cereal grain, eggs, milk, green leaves, roots, tubers and liver.

Physical properties

M. Pt. 260°C (decomp.)

Solubility Water: 1 g 1 ml⁻¹. Organic solvents: ethanol, glycerol, methanol, propylene glycol

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 8220 mg kg⁻¹ (1).

LD₅₀ intravenous, intraperitoneal mouse 89, 200 mg kg⁻¹, respectively (1,2).

LD₅₀ intravenous rabbit 117 mg kg⁻¹ (3).

Metabolism and toxicokinetics

Well absorbed from the gastro-intestinal tract, although absorption of large doses is limited. Widely distributed to most tissues and appears in breast milk. Not stored in the body to a great extent, and excess to requirement is excreted in urine (4).

Other effects

Other adverse effects (human)

Hypersensitivity reactions have occurred, ranging from very mild to, very rarely, fatal anaphylactic shock.

Other comments

Severe deficiency results in beri-beri; the acute form is characterised by cardiac failure and oedema, and the chronic form by peripheral neuritis, muscle wasting and weakness, and paralysis. In severe cases, Wernicke's encephalopathy (demyelination of the central nervous system) may develop. Disorders with peripheral resemblance to beri-beri, such as neuritis, neuralgia, cardiovascular and central nervous system diseases have been targeted for therapy with 'megadoses' of thiamine (4).

Recommended daily dietary intake is 0.8-1.1 mg for ♀ and 0.9-1.5 mg for ♂. Requirements are directly related to carbohydrate intake and metabolic rate (4).

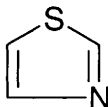
Metabolism reviewed (5).

References

1. *Int. Zeit. Vitamin.* 1967, 37, 82.

2. NTIS Report AD277-689, Natl. Tech. Inf. Ser., Springfield, VA, USA.
3. *Proc. Soc. Exp. Biol. Med.* 1948, **68**, 153.
4. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
5. Al-Rashood, K. A. M. et al *Anal. Profiles Drug Subst.* 1989, **18**, 413-458

T114 thiazole



C_3H_3NS

Mol. Wt. 85.13

CAS Registry No. 288-47-1

EINECS No. 206-021-3

RTECS No. XJ 1290000

Physical properties

B. Pt. 115-118°C Flash point 22°C Specific gravity 1.20 at 17°C

Solubility Water: slightly soluble

Occupational exposure

UN No. 1993

Ecotoxicity

Invertebrate toxicity

EC₅₀ (5-30 min) *Photobacterium phosphoreum* 13.5 ppm Microtox test (1).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431

T115 thioacetamide



C_2H_5NS

Mol. Wt. 75.13

CAS Registry No. 62-55-5

Synonyms acetothioamide; ethanethioamide; thiacetamide

EINECS No. 200-541-4

RTECS No. AC 8925000

Uses Substitute for hydrogen sulfide in the laboratory.

Physical properties

M. Pt. 113-114°C

Solubility Water: 16.3 g 100 ml⁻¹. Organic solvents: ethanol

Occupational exposure

Supply classification toxic

Risk phrases May cause cancer – Harmful if swallowed – Irritating to eyes and skin (R45, R22, R36/38)

Safety phrases Restricted to professional users – Avoid exposure – obtain special instruction before use – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S53, S45)

Environmental fate

Nitrification inhibition

75% reduction of nitrification in non-acclimated activated sludge at 0.14 mg l⁻¹ (1).

Degradation studies

Activated sludge 1000 mg l⁻¹, acclimated <1 day at 20°C, BOD 0% theoretical oxidation; 0% removed (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 30 mg kg⁻¹ (3).

LD₅₀ intraperitoneal mouse 300 mg kg⁻¹ (4).

LD_{Lo} subcutaneous mouse 2000 mg kg⁻¹ (5).

Sub-acute and sub-chronic data

Continuous administration of 10 mg kg⁻¹ intraperitoneally to rabbits caused increased concentrations of DNA and RNA in their livers after 7 wk (6).

Carcinogenicity and chronic effects

Hepatomas occurred in ♂ and ♀ mice fed 0.03% in the diet for 17 months (7).

4/56 rats fed 0.04% in the diet (average daily dose 4 mg day⁻¹) for up to 495 days developed hepatomas, two of which showed lung metastasis (8).

Rats fed 320 mg% in diet for 25 wk developed nodular cirrhosis and metastasising liver tumours (9).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537, with and without metabolic activation negative (10).

Saccharomyces cerevisiae C658-K42 weakly positive (11).

Induced cytoplasmic petite mutations in *Saccharomyces cerevisiae* (metabolic activation unspecified) (12).

Syrian hamster cell transformation assay and Rauscher murine leukaemia virus-infected Fischer 344 rat embryo cell assay positive (13).

Legislation

Land disposal prohibited under US Federal Resource Conservation and Recovery Act (14).

Other comments

Genotoxicity reviewed (15).

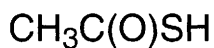
Health hazards in inorganic chemicals laboratories discussed (16).

References

1. Meinck, F. et al *Les Eaux Residuaries Industrielles* 1970.
2. Ludzack, F. J. et al *J. Water Pollut. Control Fed.* 1960, **32**, 1173.
3. *Toxicol. Appl. Pharmacol.* 1974, **27**, 380.
4. *NTIS Report AD277-689*, Natl. Tech. Inf. Ser., Springfield, VA, USA.
5. *Arch. Int. Pharmacodyn. Ther.* 1904, **12**, 447.
6. Khan, M. et al *Pak. J. Zool.* 1987, **19**(4), 439-441.
7. Gothoskar, S. V. et al *Br. J. Cancer* 1970, **24**, 498-503.
8. Dasgupta, A. et al *Oncology* 1981, **38**, 249-253.

9. Gupta, D. N. *J. Pathol. Bacteriol.* 1956, **72**, 415-426.
10. McCann, J. et al *Proc. Natl. Acad. Sci.* 1975, **72**(12), 5135-5139.
11. Morita, T. et al *Chem. Pharm. Bull.* 1989, **37**(2), 407-409.
12. Egilsson, V. et al *Mol. Gen. Genet.* 1979, **174**, 39-46.
13. Dunkel, V. C. et al *J. Natl. Cancer Inst.* 1981, **67**, 1303-1315.
14. *Fed. Regist.* 1991, **56**(21), 3864-3928.
15. Arui, P. *Mutat. Res.* 1989, **22**(2), 153-162.
16. Elo, H. *J. Chem. Educ.* 1987, **64**(6), A144-A146

T116 thioacetic acid



$\text{C}_2\text{H}_4\text{OS}$

Mol. Wt. 76.12

CAS Registry No. 507-09-5

Synonyms acetyl mercaptan; ethanethioic acid; ethanethiolic acid; methanecarbothiolic acid; thiacetic acid; thiolacetic acid; thionoacetic acid

EINECS No. 208-063-8

RTECS No. AJ 5600000

Physical properties

M. Pt. $<-17^\circ\text{C}$ **B. Pt.** 93°C **Specific gravity** 1.075 at 10°C with respect to water at 4°C

Solubility Water: soluble. Organic solvents: miscible with diethyl ether, ethanol

Occupational exposure

UN No. 2436 HAZCHEM Code 2WE Conveyance classification flammable liquid

Mammalian & avian toxicity

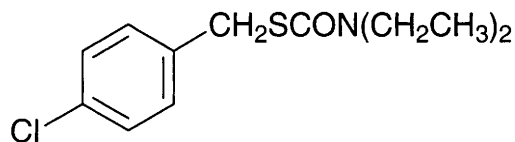
Acute data

LD_{50} intraperitoneal mouse 75 mg kg^{-1} (1).

References

1. NTIS Report AD691-490, Natl. Tech. Inf. Ser., Springfield, VA, USA

T117 thiobencarb



$C_{12}H_{16}ClNOS$

Mol. Wt. 257.78

CAS Registry No. 28249-77-6

Synonyms benthicarb; S-(4-chlorobenzyl)-N,N-diethylthiocarbamate; S-[(4-chlorophenyl)-methyl]diethylcarbamothioate; diethylcarbamothioic acid, S-[(4-chlorophenyl)methyl] ester

EINECS No. 248-924-5

RTECS No. EZ 7260000

Uses Herbicide.

Physical properties

M. Pt. 3.3°C B. Pt. 126-129°C at 0.008 mmHg Specific gravity 1.145-1.180 at 20°C

Partition coefficient $\log P_{ow}$ 3.42 (1) Volatility v.p. 1.6×10^{-2} mmHg at 23°C

Solubility Water: 30 mg l⁻¹ at 20°C. Organic solvents: acetone, benzene, ethanol, hexane, xylene

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed (R22)

Safety phrases Keep out of reach of children (if sold to general public) (S2)

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) carp, goldfish 3.6 mg l⁻¹ (2,3).

Invertebrate toxicity

LC₅₀ (96 hr) *Mysidopsis bahia* 0.37 mg l⁻¹ (4).

LC₅₀ *Daphnia pulex* 0.75 mg l⁻¹ (3).

LC₅₀ (96 hr) *Skeletonema costatum* 0.29 mg l⁻¹ (4).

LC₅₀ (oral) >100 µg bee⁻¹ (2).

Bioaccumulation

Thiobencarb uptake, depuration rates and bioconcentration factors (BCF) were measured for the bivalve *Corbicula leana* and the river snail *Cipangopludina chinensis* under field conditions (Kokai river, Japan) during 1992/1993.

Values were also estimated from a one-compartment model. Field values *Corbicula leana* 1992 [1993]: uptake rate constant 99 [183] ml g⁻¹ day⁻¹, depuration rate constant 0.055 [0.06] day⁻¹, BCF 1800 [3050]. Laboratory estimates from a first-order one-compartment model: *Corbicula leana* uptake rate constant 140 ± 74 ml g⁻¹ day⁻¹, depuration rate constant 0.049 day⁻¹, BCF 2850 ± 1500, *Cipangopludina chinensis* uptake rate constant 28 ± 13 ml g⁻¹ day⁻¹, depuration rate constant 0.22 day⁻¹, BCF 127 ± 59 (5).

Environmental fate

Degradation studies

Soil t_{1/2} under anaerobic conditions 6-8 months (1).

Primarily degraded by microbes, with little loss from volatilisation and photodegradation; t_{1/2} 2-3 wk under aerobic conditions (1).

Biodegradation was investigated under aerobic and anaerobic conditions: a substrate of non-acclimated microbes in activated sludge, field soil and river sediment was inoculated with 2 ppm thiobencarb. Degradation constants

under aerobic and anaerobic conditions were 0.54 and 0.29, respectively. When glucose and peptone were added degradation constants were 0.69 and 0.75 for aerobic and anaerobic conditions, respectively (6).

Adsorption and retention

Readily adsorbed by soil and not readily leached (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral bobwhite quail, mallard duck 7800, 10,000 mg kg⁻¹, respectively (1).

LD₅₀ dermal rabbit, rat >2000 mg kg⁻¹ (1).

LC₅₀ (1hr) inhalation rat 43 mg l⁻¹ (1).

LD₅₀ oral mouse, rat 560, 1903 mg kg⁻¹, respectively (7,8).

Carcinogenicity and chronic effects

In 2-year feeding trials, NOEL for ♂ rats was 0.9 mg kg⁻¹ day⁻¹, for ♀ rats 1.0 mg l⁻¹ day⁻¹ (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (9).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (10).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (11).

WHO Toxicity Class II (12).

EPA Toxicity Class III (2).

ADI 0.009 mg kg⁻¹ (2).

Other comments

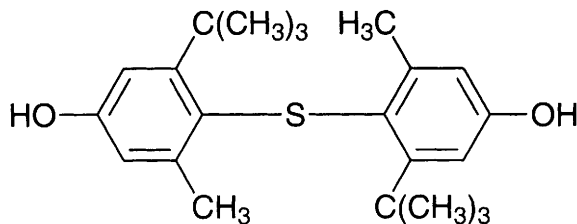
Metabolised by S-oxygenation to the corresponding sulfoxide by liver microsomes from striped sea bass (13).

Metabolic pathways reviewed (14).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
3. Hashimoto, Y. et al *J. Pestic. Sci.* 1981, **6**, 257.
4. Borthwick, P. W. et al *EPA-600/4-81-076*, 1981.
5. Uno, S. et al *Aquat. Toxicol.* 1997, **39**, 23-43.
6. Kanazawa, J. *Environ. Monitor. Assess.* 1987, **9**, 57-70.
7. *Guide to the Chemicals Used in Crop Protection* 1968, Info. Canada, Ottawa, ON, Canada.
8. *Farm Chemicals Handbook* 1983, C233, Meister Publishing, Willoughby, OH, USA.
9. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
10. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
11. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; *6th Amendment EEC Directive* 79/831/EEC; *7th Amendment EEC Directive* 91/32/EEC 1991, HMSO, London, UK.
12. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
13. Cashmann, J. R. et al *Chem. Res. Toxicol.* 1990, **3**, 433.
14. Roberts, T. R. et al (Eds.) *Metabolic Pathways of Agrochemicals. Part 1: Herbicides and Plant Growth Regulators* 1998, The Royal Society of Chemistry, Cambridge, UK

T118 4,4'-thiobis(5-*tert*-butyl-*m*-cresol)



C₂₂H₃₀O₂S

Mol. Wt. 358.54

CAS Registry No. 96-69-5

Synonyms bis(2-*tert*-butyl-4-hydroxy-6-methylphenyl) sulfide; 4,4'-thiobis(2-*tert*-butyl-6-methylphenol); 4,4'-thiobis(6-*tert*-butyl-3-methylphenol); 1,1'-thiobis(2-methyl-4-hydroxy-6-*tert*-butylbenzene)

EINECS No. 202-525-2

RTECS No. GP 3150000

Uses In rubber manufacturing.

Physical properties

M. Pt. 163-165°C

Occupational exposure

FR-VME 10 mg m⁻³

UK-LTEL 10 mg m⁻³

US-TWA 10 mg m⁻³

UK-STEL 20 mg m⁻³

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal mouse 50 mg kg⁻¹ (1).

Metabolism and toxicokinetics

20% and <2% of a dermal dose was absorbed by mice and rats, respectively (2).

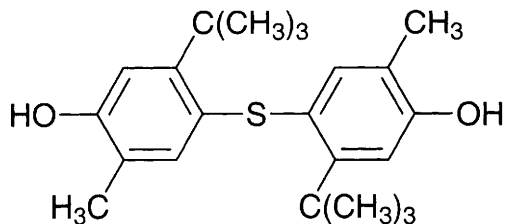
Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535 with and without metabolic activation negative (3,4).

References

1. NTIS Report AD277-689, Natl. Tech. Inf. Ser., Springfield, VA, USA.
2. Birnbaum, L. S. et al *Toxicol. Lett.* 1987, 37(1), 13-19.
3. Yamaguchi, T. et al *Eisei Kagaku* 1991, 37(1), 6-13.
4. Zeiger, E. et al *Environ. Mol. Mutagen.* 1987, 9(Suppl. 9), 1-109

T119 4,4'-thiobis(5-*tert*-butyl-*o*-cresol)



$C_{22}H_{30}O_2S$

Mol. Wt. 358.54

CAS Registry No. 96-66-2

Synonyms 4,4'-thiobis[3-(1,1-dimethylethyl)-6-methylphenol]

EINECS No. 202-522-6

RTECS No. GP 3200000

Physical properties

M. Pt. 150°C Specific gravity 1.10

Mammalian & avian toxicity

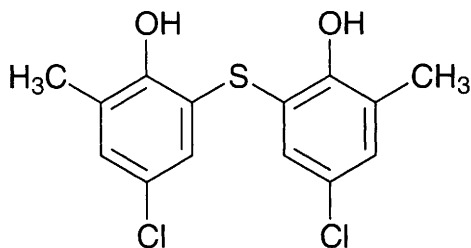
Acute data

LD₅₀ oral mammal (species unspecified) 6340 mg kg⁻¹ (1).

References

1. *Rubber Chem. Technol.* 1972, 45, 627

T120 6,6'-thiobis(4-chloro-*o*-cresol)



$C_{14}H_{12}Cl_2O_2S$

Mol. Wt. 315.22

CAS Registry No. 4418-66-0

Synonyms 2,2'-thiobis(4-chloro-6-methylphenol); Orbisan

EINECS No. 224-582-2

RTECS No. GP 3325000

Physical properties

M. Pt. 145°C (crystals from aqueous acetic acid)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1.3 mg kg⁻¹ (1).

LD₅₀ intraperitoneal rat 850 µg kg⁻¹ (1).

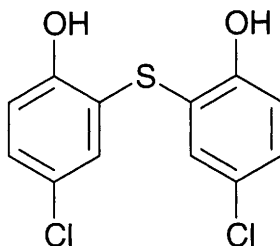
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phenols: maximum admissible concentration 0.5 µg l⁻¹, excluding natural phenols which do not react to chlorine (2).

References

1. *Pesticide Chemicals Official Compendium* 1966, 266.
2. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T121 2,2'-thiobis(4-chlorophenol)



C₁₂H₈Cl₂O₂S

Mol. Wt. 287.17

CAS Registry No. 97-24-5

Synonyms bis[2-hydroxy-5-chlorophenyl] sulfide; 2,2'-dihydroxy-5,5'-dichlorodiphenyl sulfide; fentichlor

EINECS No. 202-568-7

RTECS No. SN 0350000

Uses Anti-infective, fungicide.

Physical properties

M. Pt. 175°C

Solubility Organic solvents: benzene, ethanol

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535 with and without metabolic activation negative (1).

Other effects

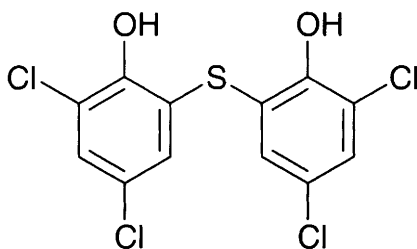
Other adverse effects (human)

Photosensitivity reported (2).

References

1. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-157.
2. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK

T122 2,2'-thiobis(4,6-dichlorophenol)



$C_{12}H_6Cl_4O_2S$

Mol. Wt. 356.06

CAS Registry No. 97-18-7

Synonyms Bidiphen; Bisoxyphe; Bitionol; CP3438; Lorotheidol; Neopellis; Vancide BL

EINECS No. 202-565-0

RTECS No. SN 0525000

Uses Sunscreen.

Physical properties

M. Pt. 187-188°C Specific gravity 1.61 at 25°C Volatility v.p. 1.1×10^{-9} mmHg at 37°C

Solubility Organic solvents: acetone

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 7 mg kg⁻¹ (1).

LD₅₀ oral mouse 760 mg kg⁻¹ (2).

LD₅₀ intraperitoneal mouse 100 mg kg⁻¹ (3).

LD₅₀ intravenous mouse 18 mg kg⁻¹ (4).

Other effects

Any other adverse effects

♀ BALB/c mice (24 hr) 10% concentration 6.0 or 0.3 J cm⁻² UVA or UVB, respectively, produced 3.4×10^{-2} and 0.3×10^{-2} mm swellings in the ear (5).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phenols: maximum admissible concentration 0.5 µg l⁻¹, excluding natural phenols which do not react to chlorine (6).

References

1. MacDougal, J. R. *Compilation of LD₅₀ values of New Drugs* 1982, 6, 612.
2. *Drugs in Japan. Ethical Drugs* 6th ed., 1982, 612, Yakugyo Jiho Co., Toyko, Japan.
3. NTIS AD277-689 Natl. Tech. Inf. Ser., Springfield, VA, USA.
4. US Army Res. Devel. Command NX 01763, NIOSH Exchange Chemicals.
5. Gerberick, G. F. et al *Food Chem. Toxicol.* 1989, 27(12), 813-819.
6. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T123 thiocarbanilide



$C_{13}H_{12}N_2S$

Mol. Wt. 228.32

CAS Registry No. 102-08-9

Synonyms diphenylthiourea; DFT; *N,N'*-diphenylthiocarbamide; sulfocarbanilide; *sym*-diphenylthiourea

EINECS No. 203-004-2

RTECS No. FE 1225000

Uses Vulcanising accelerator. Sulfur dyes.

Physical properties

M. Pt. 154°C B. Pt. decomp. Specific gravity 1.32 at 25°C

Solubility Water: insoluble. Organic solvents: chloroform, diethyl ether, ethanol

Ecotoxicity

Invertebrate toxicity

EC₅₀ (15 min) *Photobacterium phosphoreum* 9.97 pmm Microtox test (1).

Mammalian & avian toxicity

Acute data

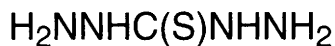
LD_{Lo} oral cat, rabbit 720, 1500 mg kg⁻¹, respectively (2,3).

LD₅₀ intraperitoneal mouse, rat 500, 1000 mg kg⁻¹, respectively (4,5).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, 26(3), 361-431.
2. Hanzlik, P. J. et al *J. Pharmacol. Exp. Ther.* 1921, 17, 349.
3. *Merck Index* 11th ed., 1989, Merck & Co., Rahway, NJ.
4. *NTIS Report* AD277-689, Natl. Tech. Inf. Ser., Springfield, VA.
5. *Med. Prac.* 1965, 16, 35

T124 thiocarbazide



CH_6N_4S

Mol. Wt. 106.15

CAS Registry No. 2231-57-4

Synonyms thiocarbonyldihydrazide; carbonothioic dihydrazide; hydrazinecarbohydrazonothioic acid; TCH; thiocarbonic dihydrazide; thiocarbonohydrazide

EINECS No. 218-769-8

RTECS No. FF 2975000

Physical properties

M. Pt. 171°C

Occupational exposure

UN No. 2811

Mammalian & avian toxicity

Acute data

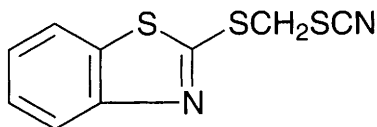
LD_{Lo} oral mouse 10 mg kg⁻¹ (1).

LD_{Lo} intraperitoneal mouse 5 mg kg⁻¹ (2).

References

1. *Natl. Acad. Sci.* 1953, 5, 44.
2. *NTIS Report AD277-689*, Natl. Tech. Inf. Ser., Springfield, VA, USA

T125 2-(thiocyanatomethylthio)benzothiazole



C₉H₆N₂S₃

Mol. Wt. 238.36

CAS Registry No. 21564-17-0

Synonyms TCMTB; thiocyanuric acid, (2-benzothiazolyl(thio))methyl ester; benthiazole; 2-[(thiocyanatomethyl)thio]benzothiazole

EINECS No. 244-445-0

RTECS No. XK 8150000

Uses Microbiocide.

Occupational exposure

Supply classification very toxic, dangerous for the environment

Risk phrases Harmful if swallowed – Very toxic by inhalation – Irritating to eyes and skin – May cause sensitisation by skin contact – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R22, R26, R36/38, R43, R50/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – After contact with skin, wash immediately with plenty of water – Wear suitable protective clothing and gloves – In case of insufficient ventilation, wear suitable respiratory equipment – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S28, S36/37, S38, S45, S60, S61)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) harlequin fish 0.036 mg l⁻¹ (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 445 mg kg⁻¹ (2).

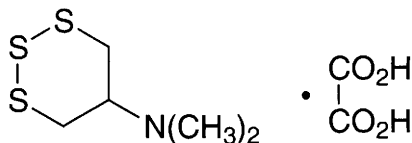
LD₅₀ oral duck, rat 1310, 1590 mg kg⁻¹, respectively (2).

LD₅₀ dermal rat, rabbit <5, 10 g kg⁻¹, respectively (2).
LD₅₀ intraperitoneal rat, mouse 73, 143 mg kg⁻¹, respectively (2).

References

1. Tooby, T. E. et al *Chem. Ind.* 1975, **21**, 523-525.
2. Lewis, R. J. (Ed.) *Sax's Dangerous Properties of Industrial Materials* 8th ed., 1992, Van Nostrand Reinhold, New York, NY, USA

T126 thiocyclam hydrogen oxalate



C₇H₁₃NO₄S₃

Mol. Wt. 271.38

CAS Registry No. 31895-22-4

Synonyms 5-dimethylamino-1,2,3-trithianyl hydrogen oxalate; *N,N*-dimethyl-5-amino-1,2,3-trithianyl ethanedioate; *N,N*-dimethyl-1,2,3-trithian-5-amine hydrogen oxalate; *N,N*-dimethyl-1,2,3-trithian-5-ylammonium hydrogen oxalate

EINECS No. 250-859-2

RTECS No. VL 8300000

Physical properties

M. Pt. 125-128°C (decomp.) **Specific gravity** 0.6 **Partition coefficient** log P_{ow} -0.07

Volatility v.p. 4.09 × 10⁻⁶ mmHg (20°C)

Solubility Water: 16.3 g l⁻¹ (pH 6.8, 20°C). Organic solvents: acetone, acetonitrile, dimethyl sulfoxide, ethanol, methanol

Occupational exposure

Supply classification harmful

Risk phrases Harmful in contact with skin and if swallowed (R21/22)

Safety phrases Keep out of reach of children (if sold to general public) – Wear suitable protective clothing and gloves – If swallowed seek medical advice immediately and show this container or label (S2, S36/37, S46)

Mammalian & avian toxicity

Acute data

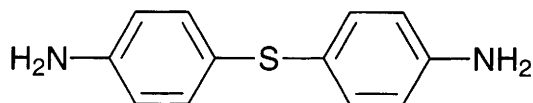
LD₅₀ oral rat, mouse, dog 195, 273, 1000 mg kg⁻¹, respectively (1,2).

LD₅₀ dermal rat 1000 mg kg⁻¹ (3).

References

1. *Khim. Se. Khoz.* 1978, **16**(2), 59.
2. *Spec. Publ. Entomol. Soc. Am.* 1978, **78**-1 24.
3. *Farm Chemicals Handbook* 1983, C234, Meister Publishing, Willoughby, OH, USA

T127 4,4'-thiodianiline



C₁₂H₁₂N₂S

Mol. Wt. 216.31

CAS Registry No. 139-65-1

Synonyms bis(*p*-aminophenyl) sulfide; *p,p'*-diaminodiphenyl sulfide; di(*p*-aminophenyl) sulfide; thioaniline; 4,4'-thiobisbenzenamine; thiodi-*p*-phenylenediamine

EINECS No. 205-370-9

RTECS No. BY 9625000

Uses Intermediate in dye manufacture.

Physical properties

M. Pt. 108°C

Solubility Water: sparingly soluble. Organic solvents: diethyl ether, ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 620, 1100 mg kg⁻¹, respectively (1).

Carcinogenicity and chronic effects

Limited evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2B (2).

The National Toxicology Program tested 4,4'-thiodianiline via feed, clear evidence of carcinogenicity in rats and mice. Increased incidence of hepatocellular carcinomas and metastases in lungs and kidneys were reported in mice. The mice were fed 2500-5000 mg kg⁻¹ diet, 5 days wk⁻¹ for 77-79 wk. In rats, increased incidences of follicular cell carcinomas of the thyroid and uterine adenocarcinomas occurred in ♀, squamous cell carcinomas or papillomas of the ear canal in ♂, and metastases in lungs of both sexes. The rats were fed 1500-3000 mg kg⁻¹ diet, 5 days wk⁻¹ for 68-72 wk (3).

Teratogenicity and reproductive effects

Oral administration of 50 mg kg⁻¹ on days 1-5 of pregnancy slightly reduced foetal implantation in mice (4).

Genotoxicity

Salmonella typhimurium TA100 with metabolic activation positive (5).

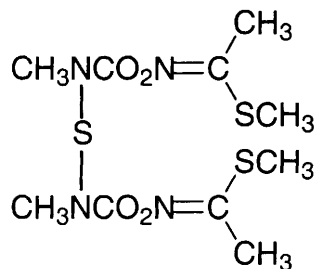
Other comments

Carcinogenicity reviewed (6).

References

1. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
2. IARC Monograph 1987, **Suppl. 7**, 56.
3. National Toxicology Program Research and Testing Division 1992, Report No. TR-47, NIEHS, Research Triangle Park, NC, USA.
4. Kamboj, V. P. et al *Indian J. Exp. Biol.* 1966, **4**, 120-121.
5. Lavoie, E. et al *Mutat. Res.* 1979, **67**(2), 123-131.
6. IARC Monograph 1982, **27**, 147-154

T128 thiodicarb



C₁₀H₁₈N₄O₄S₃

Mol. Wt. 354.48

CAS Registry No. 59669-26-0

Synonyms 3,7,9,13-tetramethyl-5,11-dioxa-2,8,14-trithia-4,7,9,12-tetra-azapentadeca-3,12-diene-6,10-dione; dimethyl *N,N'*-[thiobis[(methylimino)carbonyloxy]]bis(ethanimidothioate); Genesis; Larvin; Nivral; Securex; Semevin; Skipper; Sloggy

EINECS No. 261-848-7

Uses Insecticide, molluscicide.

Physical properties

M. Pt. 173-174°C (crystals) **Specific gravity** 1.44 g ml⁻¹ at 20°C **Volatility** v.p. 4.3 × 10⁻⁵ at 20°C

Solubility Water: 35 mg l⁻¹ at 25°C. Organic solvents: acetone, dichloromethane, methanol, xylene

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bluegill sunfish, rainbow trout 1.21, 2.55 mg l⁻¹, respectively (1).

Invertebrate toxicity

EC₅₀ (48 hr) *Daphnia magna* 0.053 mg l⁻¹ (1).

Moderately toxic to bees exposed to direct spray (1).

Environmental fate

Degradation studies

Rapidly degraded in soil under both aerobic and anaerobic conditions. DT₅₀ in soil 3-8 days, depending on soil type (1).

Abiotic removal

Rapidly hydrolysed at pH 9, slowly at pH 3 (DT₅₀ ~9 days). Aqueous suspensions are decomposed by sunlight (1).

Mammalian & avian toxicity

Acute data

Oral LD₅₀ Japanese quail 2023 mg kg⁻¹ (1).

Dietary LC₅₀ mallard duck 5620 mg kg⁻¹ diet (1).

LD₅₀ oral rat 66 (in water), 120 (in corn oil) mg kg⁻¹ (1).

LC₅₀ inhalation rat 1.5-2.2 µg l⁻¹ air (1).

LD₅₀ dermal rabbit >2000 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

Virgin ♀ albino mice were dosed orally on alternate days with 1.65, 4.13, or 8.25 mg kg⁻¹ thiocarb for 1 or 2 months. Liver weights were significantly decreased for all groups of mice, except those administered the low

dose. At the end of treatment the ♀s were mated with healthy ♂s. With the exception of low-dose treatment for 1 month and medium-dose treatment for 2 months, liver weights were significantly decreased in these pregnant mice. Newly born offspring suffered decreased liver weights. The treatment also caused a dose-related chondrodystrophy of the femoral neck in virgin and pregnant mice (2,3).

Albino rats dosed orally for 90 days with 19.91 or 39.80 mg kg⁻¹ showed increased alanine and aspartate aminotransferases and alkaline phosphatase activities. Urea and creatinine concentrations were significantly increased and total lipids and cholesterol were significantly decreased. Degenerative changes and necrosis occurred in the liver, kidney, cardiac muscles, cerebrum and cerebellum. No haematological changes were seen (4).

Carcinogenicity and chronic effects

No-observed-effect level (2 yr) for rats and mice 3 mg kg⁻¹ diet (1).

Teratogenicity and reproductive effects

Pregnant ♀ albino rats administered oral doses of 3.98 and 1.99 mg kg⁻¹ daily during days 6-15 of gestation showed decreased numbers of implantation sites and surviving foetuses, and an increased number of resorbed foetuses. Foetuses showed many visceral and skeletal malformations. ♂ Albino rats administered oral doses 3.98 and 1.99 mg kg⁻¹ daily for 65 days suffered a decrease in sperm cell count, sperm motility, and of the live/dead sperm ratio (5).

Metabolism and toxicokinetics

Rapidly degraded to methomyl in rats, and further rapidly metabolised to the unstable intermediates methomyl methylol, oxime, sulfoxide, and sulfoxide oxime. These were converted into acetonitrile and carbon dioxide, which were eliminated mainly by respiration and in the urine (6).

Irritancy

Slightly irritating to the eyes and skin of rabbits (1).

Legislation

S.I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK (7).

EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg (8).

WHO Toxicity Class II (9).

EPA Toxicity Class II (formulation) (1).

ADI (JMPR) 0.03 mg kg⁻¹ body weight (1).

Other comments

Thiodicarb inhibited the acetylcholinesterase activity of earthworm homogenates (10).

Major metabolites in plants include thiodicarb methomyl, acetonitrile, and carbon dioxide (1).

Non-phytotoxic when used as directed (1).

References

1. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
2. Abou-Egla, M. H. et al *J. Environ. Sci. (Mansoura, Egypt)* 1995, **10**(2), 49-67.
3. Abou-Egla, M. H. et al *J. Environ. Sci. (Mansoura, Egypt)* 1994, **7**, 171-190.
4. Amer, A. M. M. et al *Vet. Med. J. Giza* 1994, **42**(1B), 271-276.
5. Amer, A. M. M. *Vet. Med. J. Giza* 1996, **44**(4), 663-670.
6. Huhtanen, K. et al *Pestic. Biochem. Physiol.* 1976, **6**, 571-583.
7. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
8. S.I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
9. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
10. Shaker, N. et al *Alexandria Sci. Exch.* 1986, **7**(4), 483-500

T129 2,2'-thiodiethanol



$\text{C}_4\text{H}_{10}\text{O}_2\text{S}$

Mol. Wt. 122.19

CAS Registry No. 111-48-8

Synonyms β -thiodiglycol; bis(β -hydroxyethyl) sulfide; β,β' -dihydroxydiethyl sulfide; β -hydroxyethyl sulfide; thiodiethylene glycol; 2-hydroxyethyl sulfide

EINECS No. 203-874-3

RTECS No. KM 2975000

Physical properties

M. Pt. -16°C **B. Pt.** $164\text{--}165^\circ\text{C}$ at 20 mmHg **Flash point** $>110^\circ\text{C}$ **Specific gravity** 1.1847 at 30°C with respect to water at 20°C **Volatility** v.den. 4.21

Solubility Water: miscible. Organic solvents: chloroform

Occupational exposure

Supply classification irritant

Risk phrases Irritating to the eyes (R36)

Safety phrases Keep out of reach of children (if sold to general public) (S2)

Mammalian & avian toxicity

Acute data

LD₅₀ oral guinea pig 3960 mg kg⁻¹ (1).

LD₅₀ subcutaneous rat, mouse 400 mg kg⁻¹ (2).

LD₅₀ intravenous rabbit 3000 mg kg⁻¹ (2).

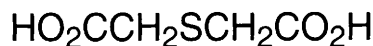
Irritancy

500 mg instilled into rabbit eye caused mild irritation (3).

References

1. *J. Ind. Hyg. Toxicol.* 1941, **23**, 259.
2. *J. Pharmacol. Exp. Ther.* 1948, **93**, 1.
3. *Union Carbide Data Sheet* 11/3/71, Union Carbide Corp., New York, NY, USA

T130 thiodiglycolic acid



$\text{C}_4\text{H}_6\text{O}_4\text{S}$

Mol. Wt. 150.16

CAS Registry No. 123-93-3

Synonyms 2,2'-thiobisacetic acid; thiodiacetic acid; (carboxymethylthio)acetic acid; dicarboxymethyl sulfide; mercaptodiacetic acid; 2,2'-thiodiethanoic acid

EINECS No. 204-663-9

RTECS No. AJ 6475000

Uses Detection of copper, lead, mercury, silver.

Physical properties

M. Pt. 128-131°C

Solubility Water: very soluble in water. Organic solvents: ethanol, hot benzene

Occupational exposure

UN No. 1940 HAZCHEM Code 2X Conveyance classification corrosive substance

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal mouse 300 mg kg⁻¹ (1).

Other effects

Any other adverse effects

Produced little or no effect when added to mouse splenic lymphocyte cultures *in vitro*, but *in vivo* administration produced apparent immune stimulation (2).

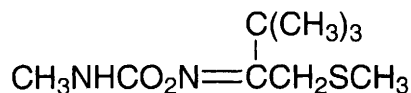
Other comments

Emits toxic fumes when heated to decomposition or on contact with acid or acid fumes.

References

1. NTIS Report AD277-689, Natl. Tech. Inf. Ser., Springfield, VA, USA.
2. Sharma, R.P. et al *Int. J. Immunopharmacol.* 1980, 2(4), 295

T131 thiofanox



C₉H₁₈N₂O₂S

Mol. Wt. 218.32

CAS Registry No. 39196-18-4

Synonyms 3,3-dimethyl-1-methylthiobutanone O-methylcarbamoyloxime; 3,3-dimethyl-1-(methylthio)-butanone-O-(N-methylcarbamoyl)oxime; 1-(2,2-dimethyl-1-methylthiomethylpropylideneamino-oxy)-N-methylformamide; 3,3-dimethyl-1-(methylthio)-2-butanone O-[(methylamino)carbonyl]oxime; Dacamox; thiofanocarb

EINECS No. 254-346-4

Uses Systemic insecticide and acaricide

Physical properties

M. Pt. 56.5-57.5°C Volatility v.p. 1.7 × 10⁻⁴ mmHg (25°C)

Solubility Water: 5.2 g l⁻¹ (22 °C). Organic solvents: readily soluble in chlorinated hydrocarbons, ketones and non-polar solvents. Slightly soluble in aliphatic hydrocarbons

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) rainbow trout, bluegill sunfish 0.13, 0.33 mg l⁻¹, respectively (1).

Invertebrate toxicity

Not toxic to honeybees when used as directed (1).

LC₅₀ (0.5% w/w thiofanox) *Helix aspersa* terrestrial snail 7.64 days (2).

Environmental fate

Degradation studies

The methylthio group is rapidly oxidised to the sulfoxide and then to the sulfone in soil. Further degradation occurs to water-soluble metabolites (1).

In soil, plants, and animals thiofanox undergoes two-step oxidation to its sulfoxide 3,3-dimethyl-1-(methylsulfinyl)-2-butanone O-[(methylamino)carbonyl]oxime and sulfone 3,3-dimethyl-1-methyl(sulfonyl)-2-butanone O[(methylamino)carbonyl]oxime (3).

Mammalian & avian toxicity

Acute data

LD₅₀ bobwhite quail, mallard duck 43, 109 mg kg⁻¹, respectively (1).

LD₅₀ oral rat 8.5 mg kg⁻¹ (4).

LD₅₀ dermal rabbit 39 mg kg⁻¹ (5).

Oral rat administered 1 mg kg⁻¹ suffered maximum inhibition of plasma cholinesterase activity and RBCs at 30 min post-dose, and maximum depression of brain cholinesterase activity 1-2 hr post-dose. In all three tissues, complete recovery of cholinesterase activity was attained at 24 hr after administration (6).

Sub-acute and sub-chronic data

No-observed-effect level (90 days) rats and beagle dogs 1 mg kg⁻¹ daily. Clinical symptoms of reversible cholinesterase inhibition were seen at 4.0 mg kg⁻¹ and lasted 3-4 hr (1).

Metabolism and toxicokinetics

Following a single dose of thiofanox, the major metabolic pathways in the rat were oxidation (40%) and *N*-demethylation (35%), with *S*-demethylation (4%) a minor pathway. The major urinary metabolite was 3,3-dimethyl-1-(methylsulfonyl)-2-butanone O-[(methylamino)carbonyl]oxime. Minor urinary metabolites identified were oxime sulfoxide, oxime sulfone, and parent sulfone. Unidentified anionic products found in the urine represented 20% of the dose (7).

Other effects

Other adverse effects (human)

Poison by ingestion and skin contact.

Legislation

WHO Toxicity Class Ib (8).

EPA Toxicity Class I (1).

Other comments

The cotyledons and developing leaves of cotton seedlings grown from thiofanox-treated cotton seeds rapidly metabolised thiofanox to its sulfoxide. The level of thiofanox in the cotton leaves declined with time, resulting in the formation of the sulfone 3,3-dimethyl-1-(methylsulfonyl)-2-butanone O-[(methylamino)carbonyl]oxime and water-soluble metabolites (9).

Less than 0.5 ppm were found of anticholinesterase carbamate residues derived from thiofanox in potato tubers harvested from plots treated with the insecticide at the 3 lb active ingredient rate. Storage of the tubers at room temperature for 10-20 weeks decreased these residues by 48-97%, through metabolic degradation; baking and frying the potatoes decreased the initial residues by 50-90%, by hydrolysis; boiling the potatoes decreased residues by 30-60%, by water extraction (10).

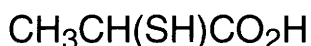
Non-phytotoxic (if used as directed) (1).

Cholinesterase inhibitor (1).

References

1. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
2. El-Wakil, H. B. et al *Alexandria Sci. Exch.* 1992, **13**(3), 497-516.
3. Chin, W.-T. et al *J. Agric. Food Chem.* 1975, **23**(5), 963-966.
4. *Agricultural Chemicals Book 1*, 1997, Thompson Publications, Fresno, CA, USA.
5. *Special Publication of the Entomological Society of America* 1978, **78-1**, 60.
6. Chin, B. H. et al *J. Agric. Food Chem.* 1980, **28**(6), 1327-1330.
7. Chin, B. H. et al *J. Agric. Food Chem.* 1980, **28**(6), 1085-1089.
8. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
9. Holm, R. E. et al *J. Agric. Food Chem.* 1975, **23**(6), 1056-1060.
10. Chin, W.-T. et al *J. Agric. Food Chem.* 1976, **24**(5), 1001-1004

T132 thiolactic acid



$\text{C}_3\text{H}_6\text{O}_2\text{S}$

Mol. Wt. 106.15

CAS Registry No. 79-42-5

Synonyms α -mercaptopropanoic acid; 2-mercaptopropionic acid; α -mercaptopropionic acid

EINECS No. 201-206-5

RTECS No. UF 5250000

Uses In depilatory and hair waving preparations.

Physical properties

M. Pt. 10°C **B. Pt.** 117°C at 16 mmHg **Specific gravity** 1.220 at 15°C with respect to water at 4°C

Solubility Water: miscible. Organic solvents: miscible with acetone, diethyl ether, ethanol

Occupational exposure

UN No. 2936 **HAZCHEM Code** 2X **Conveyance classification** toxic substance

Mammalian & avian toxicity

Acute data

LD_{50} oral rat 50 mg kg^{-1} (1).

LC_{50} (duration unspecified) inhalation rat 700 ppm (2).

Irritancy

100 μl of a 5% w/v solution instilled into rabbit eye for 24 hr caused minimal irritation (3).

Other effects

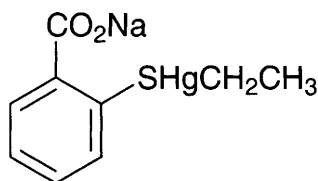
Any other adverse effects

210 $\mu\text{g ml}^{-1}$ inhibited *in vitro* growth of mouse embryo fibroblasts by 50% (3).

References

1. Patty, F. A. (Ed.) *Industrial Hygiene and Toxicology* 2nd ed., 1963, 2, 1809, John Wiley & Sons, New York, NY, USA.
2. *Report* 1971, Kodak Company, Rochester, NY, USA.
3. Bracher, M. et al *Mol. Toxicol.* 1987, **1**(4), 561-570

T133 thiomersal



C₉H₉HgNaO₂S

Mol. Wt. 404.82

CAS Registry No. 54-64-8

Synonyms mercurate(1-), ethyl[2-mercaptobenzoato(2-)-O,S]-, sodium salt; mercury, ethyl (hydrogen o-mercaptobenzoato)-, sodium salt; Elicide; mercurothiolate; Merseptyl; Nosemack; Thimerosal; Thiomersalate

EINECS No. 200-210-4

RTECS No. OV 8400000

Uses Pharmaceutic preservative. Anti-infective. Veterinary anti-bacterial, anti-fungal.

Physical properties

M. Pt. 232-233°C (decomp.)

Solubility Water: 1 g ml⁻¹. Organic solvents: ethanol

Occupational exposure

DE-MAK 0.01 mg m⁻³ (as Hg) (total dust)

JP-OEL 0.05 mg m⁻³ (as Hg)

SE-LEVL 0.03 mg m⁻³ (as Hg)

US-TWA 0.01 mg m⁻³

US-STEL 0.03 mg m⁻³

UN No. 2024 (liquid); 2025 (solid) **Conveyance classification** toxic substance

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 75, 91 mg kg⁻¹, respectively (1,2).

LD₅₀ subcutaneous rat 98 mg kg⁻¹ (3).

LD_{Lo} intravenous mouse 30 mg kg⁻¹ (4).

Sub-acute and sub-chronic data

ICR-club mice injected intraperitoneally with 1.0 ml of 0.2% buffered saline solution day⁻¹ for 7 days (close to LD₅₀ dose) showed symptoms of mercury poisoning such as incoordination and loss of control of the hind legs (5).

Teratogenicity and reproductive effects

No teratogenic effects were observed in New Zealand rabbits given 2 drops of 2% solution to both eyes 8 × on day 6 of gestation and 4 × day⁻¹ on days 7-18 gestation and sacrificed on day 29, or Wistar rats given 1.0 ml day⁻¹ of 0.2 or 2.0% solution from day 6-18 of gestation and sacrificed on day 20 (5).

Irritancy

8 µg instilled into rabbit eye (72 hr) caused mild irritation (6).

Genotoxicity

Saccharomyces cerevisiae D61.M mitotic chromosome malsegregation negative (7).

In vitro Chinese hamster cells micronucleus test negative (8).

In vitro human lymphocytes cells (48, 72 hr) gave positive results (induced micronuclei) but without a clear dose-effect relationship (9).

In vivo mouse bone marrow cells, did not induce micronuclei (10).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Sodium: guide level 20 mg l⁻¹. Mercury: maximum admissible concentration 1 µg l⁻¹ (11).
Included in Schedule 5 (Release into the Water: Prescribed Substances) Statutory Instrument No. 472, 1991 (12).

References

1. *Pesticide Chemicals Official Compendium* 1966, 1130, Association of the American Pesticide Control Officials Inc., Topeka, KS, USA.
2. *Nippon Yakurigaku Zasshi* 1962, 58, 235.
3. *Clin. Toxicol.* 1971, 4, 185.
4. *Quart. J. Pharm. Pharmacol.* 1939, 12, 212.
5. Gasset, A. R. et al *Arch. Ophthalmol.* 1975, 93, 52-55.
6. *Am. J. Ophthalmol.* 1974, 78, 98.
7. Albertini, S. *Mutagenesis* 1990, 5(5), 453-459.
8. Antoccia, A. et al *Mutagenesis* 1991, 6(4), 319-324.
9. Migliore, L. et al *Toxicol. In Vitro* 1991, 5(4), 325-326.
10. Adler, I. D. et al *Mutagenesis* 1991, 6(1), 47-53.
11. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
12. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T134 thiometon



C₆H₁₅O₂PS₃

Mol. Wt. 246.36

CAS Registry No. 640-15-3

Synonyms S-2-ethylthioethyl O,O-dimethyl phosphorodithioate; S-[2-(ethylthio)ethyl] O,O-dimethyl phosphorodithioate; Ekatin; Aseptameton; Diameaat; Ecatin; Intration; Medrin; Permutine

EINECS No. 211-362-6

RTECS No. TE 4375000

Uses Insecticide, acaricide.

Physical properties

B. Pt. 110°C at 0.1 mmHg **Specific gravity** 1.209 at 20°C **Partition coefficient** log P_{ow} 3.46

Volatility v.p. 1.725 × 10⁻⁴ mmHg at 20°C

Solubility Water: 200 mg l⁻¹ at 25°C. Organic solvents: readily soluble in common organic solvents, slightly soluble in light petroleum

Occupational exposure

Supply classification toxic

Risk phrases Harmful in contact with skin – Toxic if swallowed (R21, R25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Wear suitable protective clothing and gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S36/37, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) harlequin fish 3.2 mg l⁻¹ (1).
LC₅₀ (96 hr) carp 13.2 mg l⁻¹ (2).
LC₅₀ (96 hr) rainbow trout 8.0 mg l⁻¹ (3).
LC₅₀ (96 hr) *Saccobranchius fossilis* 11 mg l⁻¹ at 18°C (4).

Invertebrate toxicity

Toxic to bees; LD₅₀ (oral) 0.56 µg bee⁻¹ (3).

Bioaccumulation

Freshwater zebra mussels *Dreissena polymorpha* exposed to 6 mg l⁻¹ thiometon for 10 days reached body burden saturation levels of 40 mg kg⁻¹ within 7 days. Elimination of accumulated organophosphate was so low that an efficient metabolism of the pesticide was unlikely (5).

Environmental fate

Abiotic removal

Shelf-life at 20°C is ~2 years. Hydrolysed more rapidly in alkaline media than in acidic media (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 120-130 mg kg⁻¹ (2).
LD₅₀ oral mouse 25, 60 mg kg⁻¹ (6).
LD₅₀ dermal rat >1000 mg kg⁻¹ (2).

Carcinogenicity and chronic effects

No-effect level in 2-yr feeding trials in rats and dogs 2.5, 6.0 mg kg⁻¹ diet, respectively (2).

Metabolism and toxicokinetics

In animals, oxidation of the sulfur atom of the thioethyl moiety to sulfoxide, then to sulfone. Further oxidation to the corresponding phosphorothioates and phosphate, and hydrolysis to phosphoric acid (2).

Irritancy

750 µg instilled into rabbit eye caused severe irritation, 500 mg applied to rabbit skin for 24 hr caused moderate irritation (7).

Genotoxicity

Salmonella typhimurium TA1535 with metabolic activation positive, TA98, TA100, TA1538 and *Escherichia coli* WP2 *hcr* with and without metabolic activation negative (8).

Weakly mutagenic in the mouse bone marrow micronucleus test after intraperitoneal injection (9).

Weakly mutagenic in *in vivo* chromosomal aberration bioassay in rat bone marrow cells (10).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (11).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (12).

WHO Toxicity Class Ib (13).

EPA Toxicity Class II (formulation) (3).

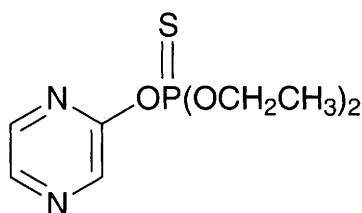
ADI (JMPR) 0.003 mg kg⁻¹ body weight (3).

References

1. Tooby, T. E. et al *Chem. Ind.* 1975, **21**, 523-525.
2. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.

3. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
4. Verma, S. R. et al *Acta Hydrobiol. Hydrochim. Ind.* 1978, **6**, 137.
5. Dauberschmidt, C. et al *Arch. Environ. Contam. Toxicol.* 1997, **33**(1), 42-46.
6. *Pesticide Chemicals Official Compendium* 1966, 1132, Assoc. Am. Pest. Control Officials, Inc., Topeka, KS, USA.
7. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
8. Moriya, M. et al *Mutat. Res.* 1983, **116**, 185-216.
9. Grover, I. S. et al *Mutat. Res.* 1985, **155**, 131-134.
10. Malhi, P. K. et al *Mutat. Res.* 1987, **188**(1), 45-51.
11. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
12. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
13. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21

T135 thionazin



$C_8H_{13}N_2O_3PS$

Mol. Wt. 248.24

CAS Registry No. 297-97-2

Synonyms phosphorothioic acid, *O,O*-diethyl *O*-pyrazinyl ester; American Cyanamid 18133; Cynophos; ethyl pyrazinyl phosphorothioate; Nemafos; Zinophos

EINECS No. 206-049-6

RTECS No. TF 5775000

Uses Superseded nematicide and insecticide.

Physical properties

M. Pt. -1.7°C **B. Pt.** 80°C **Partition coefficient** $\log P_{ow}$ 1.24 (1) **Volatility** v.p. 3×10^{-3} mmHg at 30°C
Solubility Water: slightly soluble in water. Organic solvents: miscible with most organic solvents

Occupational exposure

Supply classification very toxic

Risk phrases Very toxic in contact with skin and if swallowed (R27/28)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Wear suitable protective clothing, gloves and eye/face protection – In case of insufficient ventilation, wear suitable respiratory equipment – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S36/37/39, S38, S45)

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird 2.4 mg kg⁻¹ (3).

LD₅₀ dermal duck, pigeon, quail 1.7, 2.4, 3.2 mg kg⁻¹, respectively (4,5).

LD₅₀ oral duck, guinea pig 7, 10 mg kg⁻¹, respectively (4,6).

LD₅₀ oral rat 3.5 mg kg⁻¹ (2).

LD_{Lo} ocular rabbit 50 mg kg⁻¹ (7).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (8).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (9).

References

1. Bacci, E. et al *Environ. Sci. Technol.* 1990, **24**(6), 885-889.
2. *Toxicol. Appl. Pharmacol.* 1969, **14**, 515.
3. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
4. *Toxicol. Appl. Pharmacol.* 1979, **47**, 451.
5. ASTM Special Publication 1979, (680), 157, American Society for Testing Materials, 1916 Race St., Philadelphia, PA, USA.
6. *Guide to the Chemicals used in Crop Protection* 1973, 6, 498, Information Canada, 171 Slater St., Ottawa, ON, Canada.
7. *Pflanzenschutz- und Schaedlingsbekaempfungsmittel: Abriss einer Toxikologie und Therapie von Vergiftungen* 2nd ed., 1971, Hundt-Verlag, Hattingen, Germany.
8. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
9. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T136 thionyl chloride



Cl_2OS

Mol. Wt. 118.97

CAS Registry No. 7719-09-7

Synonyms sulfinyl chloride; sulfur chloride oxide; sulfurous dichloride; sulfurous oxychloride; sulfur oxychloride; thionyl dichloride

EINECS No. 231-748-8

RTECS No. XM 5150000

Uses In acyl chloride manufacture. Reacts with Grignard reagents to form the corresponding sulfoxide.

Physical properties

M. Pt. -104.5°C **B. Pt.** 79°C **Specific gravity** 1.638 at 20°C with respect to water at 4°C

Volatility v.p. 100 mmHg at 21.4°C

Solubility Organic solvents: miscible with benzene, carbon tetrachloride, chloroform

Occupational exposure

UK-STEL 1 ppm (4.9 mg m^{-3})

US-STEL ceiling limit 1 ppm (4.9 mg m^{-3})

UN No. 1836 **HAZCHEM Code** 4WE **Conveyance classification** corrosive substance

Supply classification corrosive

Risk phrases Reacts violently with water – Causes burns – Irritating to the respiratory system (R14, R34, R37)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S26, S45)

Mammalian & avian toxicity

Acute data

LC_{50} (1 hr) inhalation rat 500 ppm (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Chlorides: guide level 25 mg l⁻¹ (2).
Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (3).

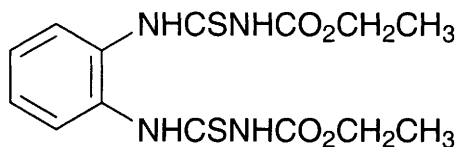
Other comments

Reviews on human health effects, physico-chemical properties, experimental toxicology, workplace exposure and ecotoxicology listed (4).

References

1. NTIS Report AD-A148-952, Natl. Tech. Inf. Ser., Springfield, VA, USA.
2. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
3. S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations 1991, HMSO, London, UK.
4. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T137 thiophanate



C₁₄H₁₈N₄O₄S₂

Mol. Wt. 370.45

CAS Registry No. 23564-06-9

Synonyms diethyl [1,2-phenylenebis(iminocarbonothioyl)]bis(carbamate); diethyl 4,4'-(*o*-phenylenebis)3-thioallophanate; Cercobin; Enorit; ethyl thiophanate; Pelt; Tapsin

EINECS No. 245-741-2

RTECS No. BA 3675000

Uses Superseded systemic fungicide. Veterinary anthelmintic.

Physical properties

M. Pt. 195°C

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat, mouse 2400, 3750 mg kg⁻¹, respectively (1).

Teratogenicity and reproductive effects

EBC is teratogenic in rats at doses of >6.8 mg kg⁻¹ (2).

Metabolism and toxicokinetics

40 mg kg⁻¹ administered orally to dairy cows was metabolised to ethyl 1*H*-benzimidazol-2-yl carbamate (EBC) which reached a maximal concentration of 0.44 µg ml⁻¹ during the first milking and was excreted by the mammary gland after 60 hr (2).

Genotoxicity

Aspergillus nidulans no significant increase in induction frequency of point mutations (3).

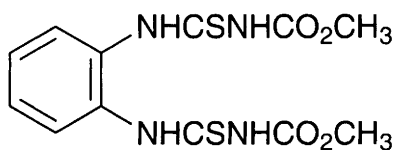
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (4).
Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (5).

References

1. Oyo Yakuri 1970, 4, 5.
2. Delatour, P. et al *Ann. Rech. Vet.* 1990, **21**(1), 87-92 (Fr.) (*Chem. Abstr.* **113**, 126006b).
3. Martinez-Rossi, N. M. et al *Mutat. Res.* 1987, **176**(1), 29-35.
4. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
5. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T138 thiophanate-methyl



C₁₂H₁₄N₄O₄S₂

Mol. Wt. 342.40

CAS Registry No. 23564-05-8

Synonyms dimethyl [1,2-phenylenebis(iminocarbonothioyl)]bis(carbamate); dimethyl 4,4'-(*o*-phenylene)bis-(3-thioallophanate); Cercobin methyl; Enorit Super; Fungo; methylthiophanate; methyltopsin; Neotopsin; Pelt 44

EINECS No. 245-740-7

Uses Fungicide.

Physical properties

M. Pt. 172°C (decomp.) **Partition coefficient** log P_{ow} 1.398 (1) **Volatility** v.p. <7.5 × 10⁻⁷ mmHg at 20°C
Solubility Water: 26.6 mg l⁻¹ at 20°C. Organic solvents: acetone, acetonitrile, chloroform, cyclohexanone, ethyl acetate, hexane, methanol

Occupational exposure

Supply classification harmful

Risk phrases Possible risk of irreversible effects (R40)

Safety phrases Keep out of reach of children (if sold to general public) – Wear suitable protective clothing and gloves (S2, S36/37)

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) rainbow trout, carp 7.8, 11 mg l⁻¹, respectively (2,3).

Midpoint cytotoxicity GF-scale cells from the scale of goldfish >400 mg l⁻¹ (4).

Invertebrate toxicity

LC₅₀ (48 hr) *Chlorella pyrenoidosa*, *Daphnia magna* 8.5, 16 mg kg⁻¹, respectively (2).

Not toxic to bees. LD₅₀ (topical) >100 µg bee⁻¹ (3).

Toxicity to other species

LC₅₀ *Rana brevipoda* tadpoles >100 ppm (duration unspecified) (5).

Environmental fate

Degradation studies

Degraded in soil, aqueous solution and under UV light by cyclisation to form carbendazim. This is then degraded to 2-aminobenzimidazole and 5-hydroxy-2-aminobenzimidazole (1).

Abiotic removal

Unstable in alkaline solution (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral Japanese quail >5000 mg kg⁻¹ (1).

LD₅₀ oral rabbit, mouse, guinea pig, rat 2270, 3400, 3640, 6640 mg kg⁻¹, respectively (6).

LD_{Lo} oral dog 4000 mg kg⁻¹ (6).

LD₅₀ intraperitoneal mouse, rat 790, 1140 mg kg⁻¹, respectively (6).

Carcinogenicity and chronic effects

In 2-yr feeding trials, no-effect level for rats and mice was 160 mg kg⁻¹ diet, and for dogs 50 mg kg⁻¹ diet (1).

Teratogenicity and reproductive effects

♂ mice were injected intraperitoneally with 8-500 mg kg⁻¹ and mated with untreated ♀ over a subsequent 8-wk period. 400-500 mg kg⁻¹ doses were toxic to ♂ but no antifertility or mutagenic effects were observed (7).

Pregnant mice were given 40, 200, 500, 1000 mg kg⁻¹ day⁻¹ orally from day 1-15 of gestation. The number of live foetuses was reduced at 1000 mg kg⁻¹, but lower doses produced no differences in implant sites, number of dead foetuses or weight of live foetuses compared with controls (7).

Metabolism and toxicokinetics

Following oral administration to rats, 61% is excreted in urine and 35% in faeces within 90 min. Metabolism involves cyclisation to carbendazim, with the principal metabolite in rats being methyl 5-hydroxybenzimidazol-2-carbamate (1).

Irritancy

Mild skin and eye irritant (species unspecified) (1).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538 with and without metabolic activation negative (8).

Escherichia coli WP2hcr with and without metabolic activation negative (9).

In vivo rat bone marrow and spermatogenic cells chromosomal aberrations negative (7).

Other effects

Any other adverse effects

1.71-34.2 g kg⁻¹ administered to rats (duration and route unspecified) caused a rapid dose-dependent fall in blood pressure which returned to normal after 10 min. 250 mg kg⁻¹ administered to rats caused a decrease in the blood coagulation time from 35 sec to 14 sec (10).

Rats, mice and guinea pigs were given 10-60 mg kg⁻¹ intraperitoneally. Decreased body temperature and spontaneous motor activity were observed in mice, but there was no effect on phenobarbitone sleeping time, forced coordinated motor response or conditioned avoidance response. In rats, no effect was observed on convulsions induced by electrical stimulation or by pentylenetetrazol. No local anaesthetic activity was observed in guinea pigs (9).

Legislation

WHO Toxicity Class Table 5 (11).

EPA Toxicity Class IV (formulation) (3).

ADI (JMPR) 0.02 mg kg⁻¹ body weight (3).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (12).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (13).

Other comments

In plants, cyclisation occurs leading to the formation of carbendazin (1).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. Canton, J. H. *Bull. Environ. Contam. Toxicol.* 1976, **16**(2), 214-218.
3. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
4. Saito, H. et al *Chemosphere* 1991, **23**(4), 525-537.
5. Nischiuchi, Y. *Sitai Kagaku* 1989, **9**(4), 23-26 (Japan.) (*Chem. Abstr.* **113**, 72754y).
6. *Toxicol. Appl. Pharmacol.* 1972, **23**, 606.
7. Makita, T. et al *Toxicol. Appl. Pharmacol.* 1973, **24**, 206-215.
8. Moriya, M. et al *Mutat. Res.* 1983, **113**, 185-216.
9. Singh, T. J. et al *Indian J. Pharmacol.* 1987, **19**, 32-36.
10. Singh, T. J. et al *Indian Vet. J.* 1989, **66**, 1116-1119.
11. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
12. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
13. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T139 thiophene



C₄H₄S

Mol. Wt. 84.14

CAS Registry No. 110-02-1

Synonyms divinylene sulfide; Huile H50; thiacyclopentadiene; thiofuran; thiofurfuran; thiole; thiotetrole

EINECS No. 203-729-4

RTECS No. XM 7350000

Uses Solvent. Manufacture of resins from thiophene-phenol mixtures and formaldehyde. Manufacture of dyes and pharmaceuticals.

Occurrence In coal tar, coal gas and technical benzene.

Physical properties

M. Pt. -38.3°C **B. Pt.** 84.4°C **Flash point** -1°C **Specific gravity** 1.057 at 25°C with respect to water at 4°C

Partition coefficient log P_{ow} 1.81 **Volatility** v.p. 40 mmHg at 12.5°C; v.den. 2.9

Solubility Organic solvents: miscible with most organic solvents

Occupational exposure

UN No. 2414 HAZCHEM Code 3WE Conveyance classification flammable liquid

Ecotoxicity

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 180 ppm Microtox test (1).

Bioaccumulation

Detected in mussels collected in two polluted bays of the Black Sea at concentrations 2.3 × those in a moderately polluted bay (2).

Environmental fate

Degradation studies

Was not biodegraded when incubated in diluted sludge at 35°C for 60 days (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird 101 mg kg⁻¹ (4).

LC_{Lo} (duration unspecified) inhalation mouse 2900 ppm (5).

LD₅₀ intraperitoneal mouse 100 mg kg⁻¹ (6).

Irritancy

Caused skin irritation and may induce sensitisation in human (7).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (8).

Other effects

Other adverse effects (human)

A woman taking thiophene in suppositories developed itching, nausea and jaundice (7).

Any other adverse effects

In rats repeated oral exposure caused effects on the liver, kidney and heart. Repeated inhalation exposure of rats, mice and rabbits affected the thyroid, liver, lung and heart and adrenals. Repeated subcutaneous injections to rats caused cellular effects in the brain (dose and duration unspecified) (7).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (9).

Other comments

Reviews on human health effects and experimental toxicology listed (10).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
2. Mironov, O. G. et al *Dopov. Akad., Nauk Ukr. RSR, Sr. B: Geol., Khim. Biol. Nauki* 1986, (10), 59-61 (Ukrain.) (*Chem. Abstr.* **106**, 38046q).
3. Battersby, N. S. et al *Appl. Environ. Microbiol.* 1989, **55**(2), 433-439.
4. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
5. Deichmann, W. B. *Toxicology of Drugs and Chemicals* 1969, Academic Press, New York, NY, USA.
6. *NTIS Report No. AD277-689*, Natl. Tech. Inf. Ser., Springfield, VA, USA.
7. *BIBRA Toxicity Profiles* 1989, British Industrial Biological Research Association, Carshalton, UK.

8. Zeiger, E. et al *Environ. Mol. Mutagen.* 1987, 9(Suppl. 9), 1-109.
9. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
10. ECETOC *Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T140 thiophosgene



CCl_2S

Mol. Wt. 114.98

CAS Registry No. 463-71-8

Synonyms carbonothioic dichloride; carbon dichlorosulfide; dichlorothiocabonyl; thiocarbonic dichloride; thiocarbonyl dichloride

EINECS No. 207-341-6

RTECS No. XN 2450000

Physical properties

B. Pt. 73.5°C **Specific gravity** 1.5085 at 15°C

Solubility Water: decomp. Organic solvents: diethyl ether

Occupational exposure

UN No. 2474 **HAZCHEM Code** 2XE **Conveyance classification** toxic substance

Supply classification toxic

Risk phrases Harmful if swallowed – Toxic by inhalation – Irritating to eyes, respiratory system and skin (R22, R23, R36/37/38)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep container tightly closed – Keep container in a well ventilated place – Wear suitable protective clothing and gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S7, S9, S36/37, S45)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 929 mg kg⁻¹ (1).

LD₅₀ intravenous mouse 100 mg kg⁻¹ (2).

Irritancy

Dermal rabbit (24 hr) 500 mg caused moderate irritation and 50 µg instilled into rabbit eye (24 hr) caused severe irritation (1).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (3).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (4).

References

1. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
2. *Report No. 04557*, US Army Armament Research and Development Command, Chemical Systems Laboratories, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD, USA.

3. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations 1991*, HMSO, London, UK.
4. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T141 thiophosphoryl chloride



Cl_3PS

Mol. Wt. 169.40

CAS Registry No. 3982-91-0

Synonyms phosphorothioic acid chloride; phosphorothionic acid trichloride; phosphorus sulfochloride; phosphorus thiochloride; trichlorophosphine sulfide

EINECS No. 223-622-6

RTECS No. XN 2930000

Physical properties

M. Pt. -40.8 to -32.6°C B. Pt. 125°C Specific gravity 1.63 at 25°C with respect to water at 4°C

Volatility v.p. 22 mmHg at 25°C ; v.den. 5.86

Solubility Organic solvents: benzene, carbon disulfide, carbon tetrachloride, chloroform

Occupational exposure

UN No. 1837 HAZCHEM Code 4XE Conveyance classification corrosive substance

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 750 mg kg⁻¹ (1).

LC₅₀ (10 min) inhalation mouse 3000 mg m⁻³ (2).

Irritancy

Irritating to skin, eyes and mucous membranes (species unspecified) (3).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Chlorides: guide level 25 mg l⁻¹ (4).

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (5).

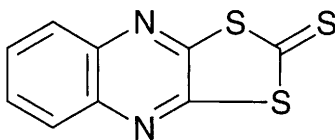
Other comments

Reviews on human health effects, experimental toxicology and environmental effects listed (6).

References

1. *J. Appl. Toxicol.* 1984, 4, 230.
2. *Progress Report NCCre* 132, June 1942, National Defense Research Committee, Office of Scientific Research and Development.
3. Sax, N. I. et al *Dangerous Properties of Industrial Materials* 8th ed., 1992, Van Nostrand Reinhold, New York, NY, USA.
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
5. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations 1991*, HMSO, London, UK.
6. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T142 thioquinox



$C_9H_4N_2S_3$

Mol. Wt. 236.34

CAS Registry No. 93-75-4

Synonyms 1,3-dithiolo[4,5-*b*]quinoxaline-2-thione; trithiocarbonic acid, cyclic 2,3-quinoxalinediyl ester; Chinothionat; Eradex; Quinothionate; Readex

EINECS No. 202-272-8

RTECS No. FG 2700000

Uses Acaricide. Fungicide.

Physical properties

M. Pt. 180°C **Volatility** v.p. 1×10^{-7} mmHg at 20°C

Solubility Organic solvents: acetone, anhydrous ethanol, kerosene, light petroleum, methanol

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed (R22)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with the skin (S2, S24)

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird 106 mg kg⁻¹ (1).

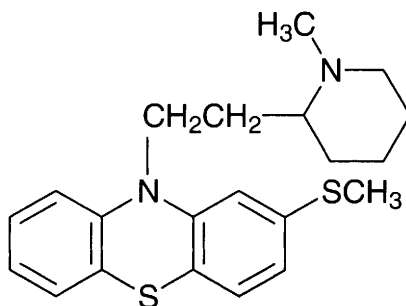
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (2).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (3).

References

1. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
2. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
3. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London

C₂₁H₂₆N₂S₂

Mol. Wt. 370.58

CAS Registry No. 50-52-2

Synonyms 10H-phenothiazine, 10-[2-(1-methyl-2-piperidyl)ethyl]-2-(methylthio)-; phenothiazine, 10-[2-(1-methyl-2-piperidyl)ethyl]-2-(methylthio)-; Mallorol; Mellaril; Mellerette; Sonapax

EINECS No. 200-044-2

RTECS No. SP 2100000

Uses Antipsychotic. Tranquiliser.

Physical properties

M. Pt. 72-74°C (crystals from acetone) B. Pt. 230°C at 0.02 mmHg

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 385, 995 mg kg⁻¹, respectively (1,2).

LD₅₀ intraperitoneal mouse, rat 65, 150 mg kg⁻¹, respectively (3,4).

LD₅₀ subcutaneous mouse, rat 310, 640 mg kg⁻¹, respectively (5,6).

Metabolism and toxicokinetics

Principal active metabolite in humans is mesoridazine, and the metabolite sulforidazine also has some toxicity (no further details given). Thioridazine and active metabolites bind to plasma proteins (7).

Other effects

Other adverse effects (human)

60% of 57 ♂ patient taking thioridazine reported sexual dysfunction compared with 25% of 64 ♂ taking other neuroleptics (8).

A 57-year old ♀ taking 150 mg day⁻¹ with occasional increases to 400 mg day⁻¹ for 6 to 8 wk (life dose 752 g) suffered blurred vision caused by pigmentary retinopathy (9).

A child who accidentally ingested 500-750 mg showed drowsiness, somnolence and hypotension (10).

Legislation

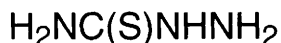
Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (11).

References

1. *Arzneim.-Forsch.* 1965, **15**, 841.
2. *Toxicol. Appl. Pharmacol.* 1971, **18**, 185.
3. *J. Med. Chem.* 1970, **13**, 23.
4. *Pharm. Chem. J. (Eng. Transl.)* 1976, **10**, 1001.
5. *Yakugaku Zasshi* 1970, **90**, 800.

6. *Med. Chem.* 1967, **4**, 199.
7. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
8. Kotin, J. et al *Am. J. Psychiatry* 1976, **133**, 82-85.
9. Lam, R. W. et al *Can. Med. Assoc. J.* 1985, **132**, 737.
10. Greenblatt, D. J. et al *Am. J. Dis. Child* 1976, **130**, 507-511.
11. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T144 thiosemicarbazide



$\text{CH}_5\text{N}_3\text{S}$

Mol. Wt. 91.14

CAS Registry No. 79-19-6

Synonyms hydrazinecarbothiamide; *N*-aminothiourea; 1-aminothiourea; isothiosemicarbazide; thiocarbamoylhydrazine

EINECS No. 201-184-7

RTECS No. VT 4200000

Uses Reagent for detection of metals.

Physical properties

M. Pt. 182-184°C

Solubility Organic solvents: ethanol

Ecotoxicity

Toxicity to other species

LC₅₀ (96 hr) *Xenopus laevis* embryos 10.97 g l⁻¹ (1).

EC₅₀ (96 hr) *Xenopus laevis* embryos 25.5 mg l⁻¹ for gross embryo malformation (1).

Environmental fate

Nitrification inhibition

0.18, 0.90 mg l⁻¹ inhibited NH₃ oxidation by 75% in activated sludge and by 50% in pure culture, respectively (2,3).

0.091, 0.455, and 0.910 mg l⁻¹ inhibited nitrification in activated sludge by 0%, 31% and 66%, respectively (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 9160 µg kg⁻¹ (5).

LD₅₀ oral dog, cat, mouse 10, 20, 94 mg kg⁻¹, respectively (6-8).

LD₅₀ intraperitoneal mouse, guinea pig 1, 24 mg kg⁻¹, respectively (7,9).

LD₅₀ subcutaneous mouse 16,407 µg kg⁻¹ (10).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1537 with and without metabolic activation negative (11).

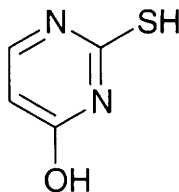
In vitro mouse, rat hepatocytes DNA repair test negative (12).

1.82 mg l⁻¹ incubated with calf thymus DNA caused 5% DNA retention alone and 60% DNA retention with CuSO₄ (13).

References

1. Dawson, D. A. et al *J. Appl. Toxicol.* 1990, **10**(1), 59-64.
2. Tomlinson, T. G. et al *J. Appl. Bacteriol.* 1966, **29**(2), 266-291.
3. Hooper, A. et al *J. Bacteriol.* 1973, **115**, 480.
4. Wood, L. B. et al *Water Res.* 1981, **15**, 543-551.
5. Lewis, R. J. (Ed.) *Sax's Dangerous Properties of Industrial Materials* 8th ed., 1992, Van Nostrand Reinhold, New York, NY, USA.
6. Saunders, W. B. *Handbook of Toxicology* 1959, **5**, 155, Philadelphia, PA, USA.
7. *Proc. Soc. Exp. Biol. Med.* 1949, **70**, 688.
8. *Arch. Environ. Contam. Toxicol.* 1985, **14**, 111.
9. NTIS Report No. AD277 689, Natl. Tech. Inf. Ser., Springfield, VA, USA.
10. *Acta Biol. Med. Germanica* 1968, **21**, 635.
11. Shimizu, H. et al *Jpn. J. Hyg.* 1978, **33**, 474-485.
12. Mori, H. et al *Jpn. J. Cancer Res. (GANN)* 1988, **79**(2), 204-211.
13. Mikelens, P. E. et al *Biochem. Pharmacol.* 1976, **25**, 821-827

T145 2-thiouracil



$C_4H_4N_2OS$

Mol. Wt. 128.15

CAS Registry No. 141-90-2

Synonyms 2,3-dihydro-2-thioxo-4(1H)-pyrimidinone; Antagothyroil; Deracil; Nobilen; thiouracil

EINECS No. 205-508-8

RTECS No. YR 1575000

Uses Treatment of hyperthyroidism, angina pectoris and congestive heart failure. Veterinary thyroid depressant, and used in hyperthyroidism to prevent fattening.

Occurrence In seeds of Brassica and Cruciferae

Physical properties

M. Pt. 300°C (decomp.)

Solubility Water: 0.05%. Organic solvents: diethyl ether, ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird 101 mg kg⁻¹ (1).

LD₅₀ oral mouse 3900 mg kg⁻¹ (2).

LD_{Lo} oral rabbit 3700 mg kg⁻¹ (3).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, limited evidence for carcinogenicity to animals, IARC classification group 3 (4).

69/81 mice administered 0.1% thiouracil in diet for up to 80 wk developed non-malignant thyroidal follicular cysts (5).

6/21 (C57xCBA)F₁ ♀ mice administered 2% in diet for 11-29 months developed hepatomas (6).

C3H and TM ♂, ♀ mice were administered 0.3% in diet for 17 months. C3H mice developed hepatomas; 12/13 ♂ and 14/16 ♀ compared with 2/32 and 0/24 controls respectively, but TM mice did not (7). Nodular hyperplasia of the thyroid was observed in Stanford albino rats administered 0.1% in diet for up to 45 wk (8). Sherman rats were administered 0.05 or 0.1% in drinking water for 35-126 wk. 11/20 developed adenomas and 1/20 developed carcinoma of the thyroid (9). 2/22 albino rats treated with 0.05% and 2% cholesterol in diet developed hepatomas after 140 wk (10).

Metabolism and toxicokinetics

Absorbed from the gastro-intestinal tract in rats and man. 30% of a 5 mg intravenous injection was recovered from rat carcasses after 3 hr, but only traces after 24 hr (11).

Oral man 100 mg was almost completely eliminated from the blood in 24 hr. 15% was broken down in the intestine, 30-50% in other tissues and body fluids and 30% was excreted unchanged in urine (11).

³⁵S-thiouracil accumulated in the thyroid 4 hr after a single intraperitoneal injection of 5 mg to Sprague-Dawley rats and reached a peak at 10 hr. Metabolites detected included ³⁵S-sulfate, protein-bound ³⁵S, unmetabolised thiouracil and two other unidentified metabolites (12).

Crosses the placenta in rabbits and dogs (13).

28-35% metabolised in rat liver homogenate preparations from ♀ Holtzman rats within 3 hr. Breakdown pathway suggested: uracil; β-ureidopropionic acid, which was further metabolised to β-alanine, ammonia and carbon dioxide (14).

Genotoxicity

In vitro mouse lymphoma L5178Y tk⁺/tk⁻ without metabolic activation negative (15).

Other effects

Other adverse effects (human)

A 56-yr-old white ♀ treated, prior to subtotal thyroidectomy, with thiouracil for 6 wk for hyperthyroidism had one small area with irregular glandular and papillary growth in each lobe interpreted as carcinoma (16).

Other comments

Reviews on human health effects and experimental toxicology listed (17).

References

1. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
2. *J. Am. Pharm. Assoc., Sci. Ed.* 1955, **44**, 56.
3. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
4. *IARC Monograph* 1987, (Suppl. 7), 72.
5. Gorbman, A. *Cancer Res.* 1947, **7**, 746-758.
6. Miller, O. J. et al *Cancer Res.* 1954, **14**, 220-226.
7. Casas, C. B. *Proc. Soc. Exp. Biol. (N.Y.)* 1963, **113**, 493-494.
8. Laqueur, G. L. *Cancer Res.* 1949, **9**, 247-255.
9. Paschkis, K. E. et al *Cancer Res.* 1948, **8**, 257-263.
10. Nelson, D. et al *Cancer Res.* 1954, **14**, 441-444.
11. Williams, R. H. et al *J. Clin. Endocrinol.* 1944, **4**, 385-393.
12. Lees, J. et al *Endocrinology* 1973, **93**, 162-171.
13. Quinones, J. D. et al *J. Nucl. Med.* 1972, **13**, 148-154.
14. Spector, E. et al *Biochem. Pharmacol.* 1959, **2**, 182-196.
15. Garberg, P. et al *Mutat. Res.* 1988, **203**(3), 155-176.
16. Crane, A. R. et al *Am. J. Pathol.* 1946, **22**, 639-640.
17. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T146 thiourea



$\text{CH}_4\text{N}_2\text{S}$

Mol. Wt. 76.12

CAS Registry No. 62-56-6

Synonyms 2-thiopseudourea; isothiurea; thiocarbamide; β -thiopseudourea; 2-thiourea

EINECS No. 200-543-5

RTECS No. YU 2800000

Uses Photographic fixing agent. Removal of stains from negatives. In resin manufacture. Vulcanisation accelerator. Reagent for bismuth and selenite.

Occurrence Occurs naturally in laburnum shrubs as a metabolite of *Verticillium albo-atrum* and *Bortrylio cinerea* (1).

Physical properties

M. Pt. 176-178°C **Specific gravity** 1.405

Solubility Water: 1 part in 11 parts at 25°C. Organic solvents: diethyl ether, ethanol

Occupational exposure

Supply classification harmful, dangerous for the environment

Risk phrases Harmful if swallowed – Possible risk of irreversible effects – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R22, R40, R51/53)

Safety phrases Keep out of reach of children (if sold to general public) – Do not breathe dust – Avoid contact with the skin – Wear suitable protective clothing and gloves – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S22, S24, S36/37, S61)

Ecotoxicity

Fish toxicity

4/20 and 12/42 rainbow trout fed 1200 ppm in diet for 15 and 20 months, respectively, developed hepatomas. The incidence of hepatomas in controls was 0/400 (2).

Invertebrate toxicity

EC₅₀ (15 min) *Photobacterium phosphoreum* 3400 ppm Microtox test (3).

Environmental fate

Nitrification inhibition

0.38, 0.76, 0.12 mg l⁻¹ inhibited nitrification in activated sludge by 0%, 72%, 75%, respectively (4,5).

76 µg l⁻¹ inhibited NH₃ oxidation in activated sludge by 75% (6).

Degradation studies

Confirmed to be non- or low-accumulative (7).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 125 mg kg⁻¹ (8).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2B (9).

Mice administered 2% thiourea in diet for up to 81 wk developed non-malignant follicular cystic changes in the thyroid (10).

21 ♀ C3H mice fed 0.25-0.375% in diet for 63 wk developed no thyroid tumours (11).

0.1% administered in drinking water to ♀ C3H mice decreased the incidence of mammary cancer from 40/96 to 5/85 (12).

♂ and ♀ C3H mice administered 0.2-0.3% in diet for 7 months resulted in hyperplastic thyroids in castrated and intact animals and 1 adenoma of the thyroid in a castrated animal (13).

10 ♂, 10 ♀ Norwegian rats and 10 ♂ Wistar rats were administered 0.25% in drinking water for 12-24 months. Of the Norwegian rats, 9 had adenomas, 1 ♂ had a carcinoma, 3 had carcinomas and adenomas and 3 had carcinomas, adenomas and foetal adenomas after 23.5 months. 5 Wistar rats had adenomas after 21.5 months and 1 had an adenoma and a foetal adenoma (14).

Osborne-Mendel rats administered 100, 250, 500, 1000 ppm in diet for 104 wk. 3/5, 4/8, 2/8 and 5/8 had liver tumours, respectively, with a 1% spontaneous incidence in controls (15).

19 ♂ rats were administered 0.2% in drinking water for up to 26 months. 1 myxomatous tumour of the nose and 17 malignant tumours involving the ear duct and orbit were observed, compared with 0 in 12 controls (16).

7/8 Hebrew University strain rats administered 0.2% in drinking water for 14-23 months developed squamous-cell carcinomas of the zymal gland and/or meibomian gland (17).

Subcutaneous ICR Swiss mice 2500 mg kg⁻¹ at 24-72 hr age caused no increase in lung adenomas, compared with controls (18).

Albino rats were given 3 doses of 3, 4, 4 ml of 10% solution intraperitoneally on 3 consecutive days, wkly for 6 months, followed by 0.2% in drinking water. 5/6 surviving rats developed tumours involving the ear duct and orbit (3 squamous-cell carcinomas) (19).

Teratogenicity and reproductive effects

Delayed hatching was observed in chick embryos treated with 2.49 mg l⁻¹ on day 17 of incubation (20).

Pregnant Swiss-Webster mice were given daily subcutaneous injections of thiourea, 5 or 10 mg kg⁻¹ for the last four days of pregnancy and the 1st 4 days post-partum, or for the 1st 4 days post-partum only. ♂ offspring of mothers treated pre- and post-partum showed decreased defensive behaviour and increased threat and attack compared with controls (21).

Metabolism and toxicokinetics

Rapidly absorbed from the gastro-intestinal tract in rats (22).

98% of radioactivity appeared in urine within 48 hr of an intraperitoneal injection of ³⁵S-labelled compound. The major product was undegraded thiourea, with small quantities of inorganic sulfate and ethereal sulfate (23).

1.95% of an intraperitoneally administered dose of ³⁵S-labelled thiourea concentrated in the thyroid of rats. Most of the ³⁵S in the gland was bound to protein or present as sulfate, whereas most in serum was present as thiourea. Desulfurated in the thyroid gland *in vitro* to produce a protein-bound sulfur molecule (24).

Readily crosses the rat placenta (25).

Sensitisation

Guinea pigs exposed to thiourea by inhalation (dose unspecified) developed allergy (26).

Occupational exposure may cause allergic dermatitis above normal levels, impaired phagocytic activity of neutrophils and IgA concentrations below those of controls (26).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100 with and without metabolic activation negative (27).

Escherichia coli PQ37 SOS Chromotest with and without metabolic activation negative (27).

Saccharomyces cerevisiae C658-K42 with metabolic activation positive, without metabolic activation negative (28).

Drosophila melanogaster zeste-white somatic mutation assay positive (29).

Other effects

Any other adverse effects

Bile and urea formation were fully inhibited in rat livers perfused for 2 hr with 50 mg 70 ml⁻¹ perfusate; enzymes from liver cytosol, microsomes, peroxisomes and lysosomes were released into the perfusate (30).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties, workplace experience, epidemiology, ecotoxicology and environmental effects listed (31).

References

1. IARC Monograph 1974, 7, 95-109.
2. Halver, J. E. Bureau of Sport Fisheries and Wild Life Research Report No. 70, 78-102, Department of the Interior, Washington, DC, USA.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, 26(3), 361-431.
4. Wood, L. B. et al *Water Res.* 1981, 15, 543-551.
5. Greenfield, J. H. et al 36th Ind. Waste Conf., Purdue University, USA, 1981, 772.
6. Tomlinson, T. G. et al *J. Appl. Bacteriol.* 1966, 29(2), 266-291.
7. *The list of existing chemicals tested on biodegradability by microorganisms or bioaccumulation in fish body* 1987, Chemicals Inspection and Testing Institute, Japan.
8. *Handbook of Toxicology* 1959, 5, 177.
9. IARC Monograph 1987, Suppl. 7, 71.
10. Gorbman, A. *Cancer Res.* 1947, 7, 746-758.
11. Dalton, A. J. et al *J. Natl. Cancer Inst.* 1948, 9, 201-223.
12. Vazquez-Lopez, E. *Br. J. Cancer* 1949, 3, 410-414.
13. Casas, C. B. et al *Endocrinology* 1952, 51, 322-328.
14. Purves, H. D. et al *Br. J. Exp. Path.* 1947, 28, 46-53.
15. Deichmann, W. B. *Toxicol. Appl. Pharmacol.* 1967, 11, 88-103.
16. Rosin, A. et al *Cancer Res.* 1957, 17, 302-305.
17. Ungar, H. et al *Toxicol. Appl. Pharmacol.* 1967, 11, 88-103.
18. Gargus, J. L. et al *Toxicol. Appl. Pharmacol.* 1969, 15, 552-559.
19. Rosin, A. et al *Cancer Res.* 1954, 14, 494-496.
20. Wittmann, J. et al *Res. Commun. Chem. Pathol. Pharmacol.* 1987, 58(2), 199-214.
21. Brain, P. F. et al *Acta Physiol. Pharmacol. Bulg.* 1986, 12(4), 3-11.
22. Wiliams, R. H. et al *Am. J. Physiol.* 1945, 143, 715-722.
23. Schulman, J. et al *J. Biol. Chem.* 1950, 183, 215-221.
24. Maloof, F. et al *J. Biol. Chem.* 1961, 236, 1689-1692.
25. Shepard, T. H. *Endocrinology* 1963, 72, 223-230.
26. Savchenko, M. V. *Gig. Sanit.* 1987, 11, 29-32 (Russ.) (*Chem. Abstr.* 108, 50965n).
27. Brams, A. et al *Toxicol. Lett.* 1987, 38(1-2), 123-133.
28. Morita, T. et al *Chem. Pharm. Bull.* 1989, 37(2), 407-409.
29. Batiste-Alentorn, M. et al *Environ. Mol. Mutagen.* 1991, 18(2), 120-125.
30. Talakin, Y. N. et al *Gig. Sanit.* 1990, 6, 60-62 (Russ.) (*Chem. Abstr.* 113, 92901x).
31. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T147 thiram



$\text{C}_6\text{H}_{12}\text{N}_2\text{S}_4$

Mol. Wt. 240.44

CAS Registry No. 137-26-8

Synonyms bis(dimethylthiocarbamoyl) disulfide; TMID; tetramethylthiuram disulfide; tetramethylthioperoxydicarbonic diamide; Akrochem TMTD; MethylTuads; Rezifilm; Tuex; Thiurad
EINECS No. 205-286-2 **RTECS No.** JO 1400000

Uses Fungicide. Seed disinfectant. Bactericide in soap. Animal repellent. Rubber accelerator and vulcaniser. Used as antiseptic.

Physical properties

M. Pt. 156°C **B. Pt.** 129°C at 20 mmHg **Specific gravity** 1.30 at 20°C **Partition coefficient** log P 1.73
Volatility v.p. 2.3×10^{-3} Pa (25°C)
Solubility Water: 30 mg l⁻¹ at 25°C. Organic solvents: acetone, chloroform, diethyl ether, ethanol

Occupational exposure

DE-MAK 5 mg m⁻³ (inhalable fraction of aerosol)

FR-VME 5 mg m⁻³

SE-LEVL 1 mg m⁻³

SE-STEL 2 mg m⁻³

UK-LTEL 5 mg m⁻³

UK-STEL 10 mg m⁻³

US-TWA 1 mg m⁻³

Supply classification harmful

Risk phrases Harmful by inhalation and if swallowed – Irritating to eyes and respiratory system – Possible risk of irreversible effects – May cause sensitisation by skin contact (R20/22, R36/37, R40, R43)

Safety phrases Keep out of reach of children (if sold to general public) – Wear suitable protective clothing and gloves (S2, S36/37)

Ecotoxicity

Fish toxicity

LC₅₀ (24, 96 hr) harlequin fish 0.02, 0.007 mg l⁻¹, respectively (1).

LC₅₀ (48 hr) rainbow trout, bluegill sunfish 0.13-0.23 mg l⁻¹ (2).

LC₅₀ (96 hr) carp 4 mg l⁻¹ (2).

LC₅₀ (96 hr) guppy 0.27 mg l⁻¹ (3).

Invertebrate toxicity

EC₅₀ (15 min) *Photobacterium phosphoreum* 0.1 ppm Microtox test (4).

EC₅₀ (96 hr) *Chlorella pyrenoidosa* 1 mg l⁻¹ (3).

EC₅₀ (48 hr) *Daphnia magna* 0.21 mg l⁻¹ (3).

LC₅₀ (96 hr) *Cloeon dipterum* 0.39-1.01 mg l⁻¹ (5).

LC₅₀ (24, 96 hr) *Gammarus pulex* 14 ppm and 0.195 ppm, respectively (6).

LC₅₀ (96 hr) *Lymnaea stagnalis* 3-35 mg l⁻¹ (6).

LC₅₀ (24, 96 hr) *Asellus aquaticus* 1882 ppm and 61 ppm, respectively (7).

Non-toxic to bees (2).

Bioaccumulation

Bioaccumulative potential of dithiocarbamates is low (8).

Environmental fate

Degradation studies

300 ppm in autoclaved and non-autoclaved alluvial sandy loam inoculated with *Pseudomonas aeruginosa* t_{1/2} 8 days, 90% decomposed in 24 days (9).

100 ppm inoculated with 30 ppm activated sludge at 25°C and pH 7 <30% degraded after 2 wk (10,11).

Major metabolites in soil are copper dimethyldithiocarbamate, dithiocarbamate, dimethylamine and carbon disulfide (12-14).

Other metabolites include elemental sulfur, methionine, formaldehyde, dimethyldithiocarbamate- α -aminobutyric acid and the corresponding keto-acid (10).

Atmospheric reaction t_{1/2} at 25°C estimated at 26.57 days, assuming ambient hydroxyl radical concentration of 8×10^5 molecule cm⁻³ (15).

Abiotic removal

Calculated bioconcentration factor 91 (16).

Adsorption and retention

Relatively immobile in loamy sand, peat moss and black clay (16).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 640 mg kg⁻¹ (17).
LD₅₀ oral mouse 1350 mg kg⁻¹ (18).
LD₅₀ oral redwing blackbird 300 mg kg⁻¹ (19).
LC₅₀ oral house sparrow 130 ppm via food (20).
LD₅₀ oral pheasant 673 mg kg⁻¹ (21).
LD₅₀ oral mallard >2800 mg kg⁻¹ (21).
LC₅₀ (4 hr) inhalation rat >0.3-1.0 mg l⁻¹ (2).
LD_{Lo} dermal rabbit 1 g kg⁻¹ (22).
LD₅₀ intraperitoneal mouse 70 mg kg⁻¹ (23).

Sub-acute and sub-chronic data

Oral rat 0, 50, 500, 1000 ppm in diet for 13 wk resulted in changes in haematological and serum biochemical parameters and gastric irritation at 500 and 1000 ppm. No-observed-effect level 50 ppm (2.5 mg kg⁻¹ day⁻¹) (24).
Oral beagle dog 0, 72, 250, 500 ppm for 13 wk, no-observed-effect level 2.2 and 2.3 mg kg⁻¹ day⁻¹ for ♂, ♀ respectively (24).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity in humans, inadequate evidence in animals, IARC classification group 3 (25).

Two-year feeding tests with 1, 10, 100, 1000 mg kg⁻¹ feed of thiram in rats did not affect clinical parameters, with the exception of the highest dose group, where low weight gains in both ♂ and ♀ and decrease in blood haemoglobin for ♀ were observed. No-effect level of 5 mg kg⁻¹ body weight was evaluated, giving tolerable daily intake of 0.05 mg kg⁻¹ (26).

Oral ♂ Wistar rats 0, 3, 30 and 300 ppm for 104 wk. 300 ppm caused muscle atrophy, chronic nephrosis and anaemia in ♀ rats, myocardial lesions in ♂ rats. Oral beagles 0, 0.4, 4 and 40 mg kg⁻¹ day⁻¹ caused vomiting, salivation, retinal lesions, anaemia, liver and kidney damage (27).

TD_{Lo} (1 yr continuous) oral rat 108 mg kg⁻¹ dermal and appendages tumours (28).

F344 rats were given thiram in diet at concentrations of 0, 0.1 and 0.05% for 104 wk; adverse effects included reduced body-weight gain and liver dysfunction, but no significant lesions or tumour induction observed. It was concluded that under these experimental conditions thiram is not carcinogenic (29).

Teratogenicity and reproductive effects

Embryotoxic in white leghorn chicken eggs (30).

TD_{Lo} (1-20 day pregnant) oral rats 420 mg kg⁻¹ developmental abnormalities observed in the newborn included cardiovascular, biochemical and metabolic effects (31).

TD_{Lo} (4-11 day pregnant) oral rats 400 mg kg⁻¹ foetotoxicity, foetal death (32).

In rams administered 12 or 30 mg kg⁻¹ day⁻¹ of thiram in their feed for 5 months, semen volume decreased and total number of spermatozoa and total number of dead and abnormal spermatozoa increased. Fertilising capacity of sperm decreased (33).

Metabolism and toxicokinetics

Metabolites include carbon disulfide, which contributes to the toxicity (2).

>83% of 125 mg kg⁻¹ administered to rats as a single oral dose was absorbed and eliminated via expired air (41-48%), urine (25-40%) and faeces (2-5%); ~3% was recovered in various organs. 84-90% was eliminated within 4 days (24).

Urinary metabolites detected included an alanine conjugate of carbon disulfide, a glucuronide conjugate of dimethyl dithiocarbamate, a thiosulfonic acid, the methyl ester of dimethyldithiocarbamate, and an alanine conjugate. These indicate that the metabolic pathway involves reduction of the disulfide bond and reactions of the thiol moiety to form oxidative and conjugative polar products (24).

5 hr after intraperitoneal administration to rats, a dose-dependent excretion of carbon disulfide was observed in expired air (34).

Irritancy

100 mg instilled into rabbit eye (24 hr) caused moderate irritation (35).

Occupational dermatosis from exposure to rubber is largely brought about by the catalysts, e.g. tetramethylthiuram and antioxidants in the rubber (36).

Application of dry powder to skin of humans produced slight erythema in 9% of cases (37).

Dermatitis from exposure to cutting oil, patch test constituents of the standard series may occur in cutting fluid but also found in rubber accelerators (38).

Sensitisation

Cross sensitivity to bisdithiocarbamates is possible (39).

Genotoxicity

Salmonella typhimurium (strain unspecified) without metabolic activation positive (40).

Escherichia coli with metabolic activation, 55% increase in phage-inhibition capacity (40).

Aspergillus nidulans without metabolic activation induced point mutations (40).

Aspergillus nidulans 20-40 ppm induced abnormal chromosome segregation (41).

Administration of 10 µg ml⁻¹ for 2 hr to Chinese hamster V79 cell line proved to be mutagenic and cytotoxic (42).

In vitro human peripheral blood lymphocytes. Dose-dependent inhibition of thymidine uptake and unscheduled DNA synthesis without metabolic activation and unscheduled DNA synthesis and increased frequency of sister chromatid exchanges with metabolic activation (43).

Increased frequency of sister chromatid exchanges in human lymphocytes with or without metabolic activation (44).

Mutagenic in micronucleus (mouse bone marrow) test after intraperitoneal injection of 14-140 mg kg⁻¹ or intragastric administration of 300-1200 mg kg⁻¹ (45).

Effects of thiram on germ cells of Swiss albino ♂ rats were evaluated by analysing spermatocytes for chromosomal aberrations and spermhead morphology assays. Doses were 80, 200 and 320 mg kg⁻¹ given by gavage in 3 consecutive daily doses. Results showed significant increases in frequency of chromosomal aberrations and abnormal sperm (46).

Mutagenic in micronucleus (mouse bone marrow) test after intraperitoneal injection of 100 mg kg⁻¹ to Swiss albino mice. A significant number of dead implants were induced when thiram was given to ♂ mice in the diet at 10% of the oral LD₅₀ during the whole spermatogenesis cycle (8 wk); this post-implantation loss indicates a dominant lethal mutation (47).

Other effects

Any other adverse effects

Induced accumulation of acetaldehyde in blood of rats receiving ethanol at the same time (48).

Gavage rats (24 hr) single dose (unspecified) caused disorder of phosphate metabolism in the kidney (49).

Toxicity greater in the presence of fats, oils and fat solvents (species unspecified) (50).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (51).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (52).

WHO Toxicity Class III (53).

EPA Toxicity Class III (37).

ADI (JMPR) 0.02 mg kg⁻¹ body weight (37).

US Office of Pesticide Programs classification pending (54).

EEC maximum residue levels strawberries, salads 3.8 ppm, other fruit and vegetables 3 ppm (2).

Other comments

- Aqueous hydrolysis of tetramethylthiuram disulfide in foods yields dimethyl dithiocarbamate and dimethylaminothioxomethylene sulfuric acid at acid pH; further hydrolysis produces CS₂, (CH₃)₂NH, and COS (55).
- Metabolism and mechanism of toxicity reviewed (56).
- Main ingredient of antiseptic spray Nobecutan (50).
- Toxicity reviewed (57,58).
- At 100 µg g⁻¹ soil microbial population suppressed by 2 log orders of magnitude (58).

References

1. Tooby, E. et al *Chem. Ind. (London)* 1975, **6**, 523-526.
2. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
3. van Leeuwen, C. J. et al *Aquat. Toxicol.* 1985, **7**(3), 145-164.
4. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
5. Seuge, J. et al *Hydrobiologia* 1983, **101**, 215.
6. Bluzat, R. et al *Environ. Pollut.* 1983, **7**, 98.
7. Seuge, J. et al *Environ. Pollut., Ser. A* 1983, **31**(3), 177-189.
8. van Leeuwen, C. J. *Environ. Contam. Int. Conf.* 2nd 1986, 215-217.
9. Shirko, C. K. et al *Bull. Environ. Contam. Toxicol.* 1985, **35**, 354-361.
10. Kawasaki, M. *Ecotoxicol. Environ. Saf.* 1980, **4**, 444-454.
11. Hutzinger, O. et al (Ed.) *Aquatic Pollutants: Transformation and Biological Effects* 1980, Pergamon, Oxford, UK.
12. Rajagopal, B. S. et al *Res. Rev.* 1984, **93**, 1-199.
13. Kumarasamy, R. et al *Chemosphere* 1976, **5**, 107-112.
14. Maeda, K. et al *Kogyo Gijutsuin Hakko Kenkyusho Kenkyo Hokoku* 1968, 108.
15. GEMS: Graphic Evaluation Modeling System. Fate of Atmospheric Pollutants database 1986, US EPA.
16. Martin, H. et al *The Pesticide Manual* 7th ed., 1983, British Crop Protection Council, Farnham, UK.
17. Gaines, *Toxicol. Appl. Pharmacol.* 1969, **14**, 515.
18. *Hyg. Sanit. (USSR)* 1964, **29**, 37.
19. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355.
20. Babu, T. H. *Pavo* 1988, **26**(1-2), 17-23.
21. *Handbook of Toxicity of Pesticides to Wildlife* 1984, U.S. Dept. Interior, Fish and Wildlife Service, Washington, DC, USA.
22. Izmerov, N. F. *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, Moscow, USSR.
23. *Drugs in Japan* 6th ed., 1982, Yakugyo Jiho Co., Tokyo, Japan.
24. *Pesticide Residues in Food – 1992 1993*, WHO, Geneva, Switzerland.
25. *IARC Monograph* 1987, **Suppl. 7**, 72.
26. Knapek, R. et al *Z. Gesamte Hyg. Ihre Grenzgeb.* 1989, **35**(6), 358-360 (Ger.) (*Chem. Abstr.* **110**, 93666z).
27. Maita, K. et al *Fundam. Appl. Toxicol.* 1991, **16**(4), 667-686.
28. *Registry of Toxic Effects of Chemical Substances* 1990, **48**, 38513.
29. Hasagawa, R. et al *Toxicology* 1988, **51**(2-3), 155-165.
30. van Leeuwen, C. J. et al *Aquat. Toxicol.* 1986, **9**(2-3), 129-145.
31. *Gig. Sanit.* 1986, **51**(6), 23 (Russ.).
32. *Bull. Exp. Biol. Med.* 1982, **93**, 107.
33. Sauov, A. et al *Biol. Immunol. Reprod.* 1987, **13**, 56-61 (Bulg.) (*Chem. Abstr.* **108**, 1849v).
34. Dalvi, R. R. et al *Pharmacol. Toxicol.* 1986, **58**, 38-42.
35. Marhold, J. V. *Sbornik Vysledku Toxikologickelo Vysetreni Latek A Pipravku* 1972, Prague, Czechoslovakia.
36. Kanerva, L. et al *Gig. Tr. Prof. Zabol.* 1987, **4**, 11-13, (Russ.) (*Chem. Abstr.* **107**, 27751k).
37. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
38. Grattan, C. E. H. et al *Contact Dermatitis* 1989, **20**(5), 372-376.
39. Lisi, P. et al *Contact Dermatitis* 1987, **17**(4), 212-218.
40. Zozienicka, M. et al *Mutat. Res.* 1981, **89**, 1-7.
41. Upshall, A. et al *Mutat. Res.* 1981, **89**, 297-301.
42. Paschin, Y. V. et al *Food Chem. Toxicol.* 1985, **23**(3), 373-375.
43. Perocco, P. et al *Teratog., Carcinog., Mutagen.* 1989, **9**(2), 75-81.
44. Pienkowska, M. et al *Mutat. Res.* 1990, **245**(2), 119-123.
45. Hu, Y. et al *Huanjing Kexue* 1987, **8**(6), 30-32 (Ch.) (*Chem. Abstr.* **108**, 107873n).

46. Prasad, M. H. et al *Food Chem. Toxicol.* 1987, **25**(9), 709-711.
47. Agrawal, R. C. et al *Food Chem. Toxicol.* 1997, **35**(5), 523-525.
48. *IARC Monograph* 1976, **12**, 225-236.
49. Garszel, J. et al *Bromatol. Chem. Toksykol.* 1986, **19**(4), 243-250 (Pol.) (*Chem. Abstr.* **107**, 34691v).
50. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
51. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
52. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Process and Substances) Regulations* 1991, HMSO, London, UK.
53. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
54. *US Office of Pesticide Programs List of Chemicals Evaluated for Carcinogenic Potential* 1996, US Environmental Protection Agency, Washington, DC 20460, USA.
55. Schmitt, A. et al *Dtsch. Lebensm.-Rundsch.* 1988, **84**(11), 347-351.
56. Dalvi, R. R. *Vet. Hum. Toxicol.* 1988, **30**(5), 480-482.
57. *Dangerous Prop. Ind. Mater. Rep.* 1990, **10**(6), 77-88.
58. Odeyemi, O. et al *Indian J. Agric. Sci.* 1988, **58**(8), 624-628

T148 thorium

Th

Th

Mol. Wt. 232.04

CAS Registry No. 7440-29-1

EINECS No. 231-139-7

RTECS No. XO 6400000

Uses In nuclear reactors. As a reducing agent in metallurgy. Catalyst in organic synthesis.

Occurrence Occurs in minerals thorite, thorianite, orangite, yttracrasite and in monazite sand. ~15 ppm in the Earth's crust.

Physical properties

M. Pt. $1842 \pm 30^\circ\text{C}$ B. Pt. $\sim 4225^\circ\text{C}$ Specific gravity 11.3-11.72

Occupational exposure

UN No. 2975 (pyrophoric)

Ecotoxicity

Bioaccumulation

Concentrated in *Euglena* sp. $\geq 10^6 \times$ aqueous abundances (1).

Mean soil:tissue concentration ratios in chicken, steer and pig 1×10^{-4} , 0.7×10^{-4} and 0.4×10^{-4} , respectively (2).

Levels of 0.77 ± 0.10 Bq kg^{-1} fresh weight found in fish from the Rhone (3).

Mammalian & avian toxicity

Metabolism and toxicokinetics

Average daily intake in urban population in Bombay of ^{232}Th was 2 μg from food, 0.03 μg from drinking water and 0.02 μg from inhalation. Concentration ranges in lungs and bones were 1.5-16 $\mu\text{g kg}^{-1}$ and 0.2-9.0 $\mu\text{g kg}^{-1}$, respectively. Average urinary concentration was 12 ng l^{-1} . Pulmonary lymph nodes had the highest concentration amongst tissues tested at 31.4-85.5 $\mu\text{g kg}^{-1}$ (4).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (5).

Other comments

Reviews on human health effects, experimental toxicology and environmental effects listed (6).

References

1. Mann, H. et al *Chem. Geol.* 1987, **63**, (1-2), 39-43.
2. Linsalata, P. et al *J. Environ. Radioact.* 1991, **14**(3), 233-257.
3. Lambrechts, A. et al *J. Environ. Radioact.* 1987, **5**(2), 105-121.
4. Sunta, C. M. et al *J. Radioanal. Nucl. Chem.* 1987, **115**(1), 149-158.
5. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
6. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T149 thorium chloride



Cl_4Th

Mol. Wt. 373.85

CAS Registry No. 10026-08-1

Synonyms tetrachlorothorium; thorium tetrachloride

EINECS No. 233-056-1

RTECS No. XO 6475000

Physical properties

M. Pt. 770°C B. Pt. 921°C Specific gravity 4.59

Solubility Water: soluble. Organic solvents: ethanol, ethylenediamine

Ecotoxicity

Invertebrate toxicity

1 g l⁻¹ had no effect on the growth of *Klebsiella oxytoca* or *Klebsiella pneumoniae* (1).

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal mouse, rat 534, 1900 mg kg⁻¹, respectively (2,3).

LD₅₀ subcutaneous mouse 4000 mg kg⁻¹ (3).

LD_{L0} intravenous rat, rabbit 15-28, 50 mg kg⁻¹, respectively (3,4).

Genotoxicity

Bacillus subtilis rec assay negative (5).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Chlorides: guide level 25 mg l⁻¹ (6).

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (7).

References

1. Wong, S. H. *Bull. Environ. Contam. Toxicol.* 1988, **40**, 525-531.
2. C. R. *Hebd. Seances Acad. Sci.* 1963, **256**, 1043.
3. *Environ. Qual. Saf. Suppl.* 1975, **1**, 1.

4. *J. Pharmacol. Ex. Ther.* 1931, **43**, 61.
5. Nishioka, H. *Mutat. Res.* 1975, **31**, 185-189.
6. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
7. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T150 thorium dioxide



O₂Th

Mol. Wt. 264.04

CAS Registry No. 1314-20-1

Synonyms thorium oxide; thoria; thorium(IV) oxide; thorotrast; Umbrathor

EINECS No. 215-225-1

RTECS No. XO 6950000

Uses Radiopaque medium used as a diagnostic aid.

Physical properties

M. Pt. 3390°C Specific gravity 10.0

Mammalian & avian toxicity

Metabolism and toxicokinetics

A sternal biopsy of a patient (aged 49 years) who had been injected with thorium dioxide at the age of 7 showed localisation in bone marrow macrophages (1).

Other effects

Other adverse effects (human)

Of 103 military personnel who had undergone angiography with thorium dioxide between 1943 and 1946, 20 developed hepatocellular carcinoma and 16 developed intrahepatic bile duct carcinoma by April 1987, whereas 67 were still alive without cancer in 1989 (2).

Seven cases of angiosarcoma of the liver were reported in patients who received intra-arterial thorotrast for radiological investigation between 1974 and 1977 (3).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (4).

Other comments

Reviews on human health effects, experimental toxicology and environmental effects listed (5).

References

1. Hallegot, P. et al *Radiat. Environ. Biophys.* 1988, **27**, 67-78.
2. Kiyosawa, K. et al *Environ. Res.* 1989, **49**(2), 166-172.
3. Baxter, P. J. et al *Br. J. Cancer* 1980, **41**, 446.
4. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
5. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T151 thorium nitrate



$\text{N}_4\text{O}_{12}\text{Th}$

Mol. Wt. 480.06

CAS Registry No. 13823-29-5

Synonyms thorium(4+) nitrate; thorium tetranitrate

EINECS No. 237-514-1

RTECS No. XO 6825000

Uses Used with 1% cerium nitrate as impregnating liquid for incandescent mantles. Reagent for fluorine determination.

Occurrence Obtained from monazite

Physical properties

Solubility Water: very soluble in water. Organic solvents: ethanol, ethers, esters, ketones

Occupational exposure

UN No. 1477

UN No. 3218 (aqueous solution) HAZCHEM Code 1 $\frac{1}{2}$ HAZCHEM Code 2 $\frac{1}{2}$ (aqueous solution)

Conveyance classification oxidising substance

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 1760 mg kg⁻¹ (1).

LD₅₀ intravenous mouse, rat 45, 47.6 mg kg⁻¹, respectively (2).

LD₅₀ intraperitoneal rat 60 mg kg⁻¹ (2).

LD_{Lo} intraperitoneal rabbit 500 mg kg⁻¹ (3).

Teratogenicity and reproductive effects

A single intratesticular injection of 38.7 mg kg⁻¹ in rats caused severe damage to the seminiferous epithelium and destroyed all spermatozoa within 2 days (4).

Metabolism and toxicokinetics

♂ Wistar rats received intravenous injection of 1 mg 2 × wk⁻¹ for 5 wk and were sacrificed 6 months after the last injection. Thorium concentrated in a non-soluble form in bone marrow macrophages, hepatocytes and Kupffer cells (5).

Genotoxicity

In vivo mouse bone marrow micronucleus test positive (6).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (7).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Nitrates: maximum admissible concentration 50 mg l⁻¹ (8).

References

1. *Can. J. Res., Sec. E. Med. Sci.* 1948, **26**, 303.
2. *Env. Qual. Saf. Suppl.* 1975, **1**, 1.
3. *Am. J. Physiol.* 1907, **18**, 426.
4. Kamboj, V. P. et al *J. Reprod. Fertil.* 1964, **7**, 21.
5. Hallegot, P. et al *Radiat. Environ. Biophys.* 1988, **27**(1), 67-78.

6. Liao, M. et al *Weisheng Dilixue Zazhi* 1988, 2(2), 83-86 (Ch.) (*Chem. Abstr.* 112, 134189h).
7. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
8. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T152 L-threonine



$\text{C}_4\text{H}_9\text{NO}_3$

Mol. Wt. 119.12

CAS Registry No. 72-19-5

Synonyms 2-amino-3-hydroxybutyric acid; 2-amino-3-hydroxybutanoic acid; α -amino- β -hydroxybutyric acid

EINECS No. 200-774-1

RTECS No. XO 8590000

Uses Essential nutritional amino acid in humans and rats. Used in biochemical research.

Occurrence Occurs in eggs, milk, casein, gelatins and other proteins.

Physical properties

M. Pt. 255-257°C (decomp.)

Environmental fate

Nitrification inhibition

3.6 mg l⁻¹ inhibited ammonia oxidation by *Nitrosomonas* sp. by 50% (1).

Degradation studies

333 mg l⁻¹ in activated sludge acclimated for 15 days, 91% removed (2).

Degraded by *Escherichia coli* enzymes threonine dehydrogenase, threonine deaminase and serine transhydroxymethylase (3).

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat 3098 mg kg⁻¹ (4).

LD₅₀ oral rat >2 g kg⁻¹ (mixture containing 52.16 g l⁻¹ threonine) (5).

Sub-acute and sub-chronic data

Repeated administration of a bactericidal preparation containing 52.16 g l⁻¹ threonine (also glycine, alanine, valine and methionine) did not retard rat growth or affect haematological indices after 1 month, but caused dystrophic changes in rat heart muscle and hepatic parenchyma, atrophy of the reticuloendothelium of the spleen and depressed thyroid activity after 2 months (5).

Carcinogenicity and chronic effects

Predicted non-carcinogenic in CASE study (6).

Metabolism and toxicokinetics

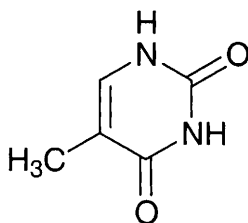
Metabolised in the liver of pigs by threonine dehydrogenase and threonine dehydratase to glycine and 2-ketobutyrate (7).

References

1. Clark, C. et al *J. Bacteriol.* 1967, 93, 1309.
2. Ludzack, F. J. et al *J. Water Pollut. Control Fed.* 1960, 32, 1173.

3. Shakalis, I. O. et al *Biotehnologiya* 1990, (2), 16-17 (Russ.) (*Chem. Abstr.* **113**, 208085r).
4. *Arch. Biochem. Biophys.* 1955, **58**, 253.
5. Tyurina, N. L. et al *Prod. Kompleksn. Pererals. Otkhodov Aminokislotnogo Proizrod. Puti Ikh Realiz.* 1990, 32-50 (Russ.) (*Chem. Abstr.* **115**, 113037d).
6. Rosenkranz, H. S. et al *Mutat. Res.* 1990, **228**(2), 105-124.
7. Ballevre, O. et al *Am. J. Physiol.* 1990, **259**(4, Pt. 1), E483-E491

T153 thymine



C₅H₆N₂O₂

Mol. Wt. 126.11

CAS Registry No. 65-71-4

Synonyms 5-methyl-2,4-(1*H*,3*H*)-pyrimidinedione; 5-methyluracil; thymine (pure base)

EINECS No. 200-616-1

RTECS No. XP 2100000

Uses Used in biochemical research.

Occurrence A pyrimidine derivative; constituent of nucleic acids. Originally isolated from thymus nucleic acid.

Physical properties

M. Pt. 335-337°C (decomp.)

Solubility Water: 4 g l⁻¹ at 25°C. Organic solvents: diethyl ether, ethanol

Environmental fate

Degradation studies

5 day BOD determined using acclimated mixed microbial cultures; predicted 2.62, 2.97 and 2.16, experimental 3.25 (1).

Degraded by *Escherichia coli* B; used as sole source of nitrogen or carbon. Degradation pathway: thymine; hydrated to dihydrothymine; hydrated to *N*-carbamoyl-β-aminoisobutyric acid; hydrolysed to β-aminoisobutyric acid, CO₂ and NH₃ (2).

Thymine is catabolised in *Burkholderia cepacia* ATTC 25416 via a reductive pathway. The first pathway enzyme, dihydropyrimidine dehydrogenase, used NADPH as its nicotinamide cofactor. The second and third pathway enzymes are dihydropyrimidinase and *N*-carbamoyl-β-alanine amidohydrolase, respectively (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 3500 mg kg⁻¹ (4).

Genotoxicity

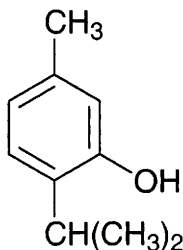
Salmonella typhimurium (strain unspecified) with and without metabolic activation negative (5).

Escherichia coli WP2 (λ) with and without metabolic activation negative (5).

References

1. Babeu, L. et al *J. Ind. Microbiol.* 1987, **2**(2), 107-115.
2. Patel, B. N. et al *Microbios* 1987, **49**(199), 107-113.
3. West, T.P. *Arch. Microbiol.* 1997, **168**(3), 237-239.
4. *J. Am. Pharm. Assoc., Sci. Ed.* 1955, **44**, 56.
5. Rossman, T. G. et al *Mutat. Res.* 1991, **260**(4), 349-367

T154 thymol



$C_{10}H_{14}O$

Mol. Wt. 150.22

CAS Registry No. 89-83-8

Synonyms 5-methyl-2-(1-methylethyl)phenol; thyme camphor; *m*-thymol

EINECS No. 201-944-8

RTECS No. XP 2275000

Uses Topical antiseptic, anthelmintic.

Occurrence Occurs in essential oils of *Thymus vulgaris* L. and *Monarda punctata*

Physical properties

M. Pt. 51.5°C B. Pt. -233°C Flash point 102°C Specific gravity 0.9699 at 25°C with respect to water at 4°C

Solubility Water: 1 g l⁻¹. Organic solvents: chloroform, diethyl ether, ethanol, glacial acetic acid, olive oil

Occupational exposure

Supply classification corrosive, dangerous for the environment

Risk phrases Harmful if swallowed – Causes burns – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R22, R34, R51/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – After contact with skin, wash immediately with plenty of water – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S26, S28, S36/37/39, S45, S61)

Ecotoxicity

Fish toxicity

LC₅₀ salmon 7.5 mg l⁻¹ (estimated; duration unspecified) (1).

Invertebrate toxicity

EC₅₀ (5 min) *Photobacterium phosphoreum* ~3.0 mg l⁻¹ (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 640, 980 mg kg⁻¹, respectively (2,3).

LD_{Lo} oral cat, rabbit 250, 750 mg kg⁻¹, respectively (4).

LD_{Lo} subcutaneous mouse, rat 800, 1600 mg kg⁻¹, respectively (4,5).

LD_{Lo} intravenous rabbit, mouse, dog 60, 100, 150 mg kg⁻¹, respectively (4,6,7).

Teratogenicity and reproductive effects

Immature ♀ rats were administered 1 mg rat⁻¹ day⁻¹ for 4 days with 10 immunising units of gonadotrophic hormone on day 2, by subcutaneous injection. Animals were sacrificed on day 5 and showed no statistically significant increase in ovarian weight, but a significant increase in uterine weight (8).

Metabolism and toxicokinetics

Absorbed from the gastro-intestinal tract and excreted unchanged and as the glucuronide (species unspecified) (9).

Irritancy

Irritating to the gastric mucosa. Fats and alcohol increase absorption and aggravate symptoms (species unspecified) (9).

Sensitisation

A contact allergy developed when thymol reacted with the degradation products of a triazine derivative, both present as preservatives in a heparinoid cream (10).

Genotoxicity

In vitro Syrian hamster embryo cells induced sister chromatid exchanges (metabolic activation unspecified) (11).

Laboratory animals treated with thymol for 48 hr had morphological cell transformation initiated by DNA synthesis (11).

Growth of mammalian V79 cells was completely inhibited by 30 µg l⁻¹ for 24-48 hr. Cells exposed to 30-300 µg l⁻¹ for 2 hr showed concentration-dependent inhibition of DNA-, RNA- and protein-synthesis (12).

Other comments

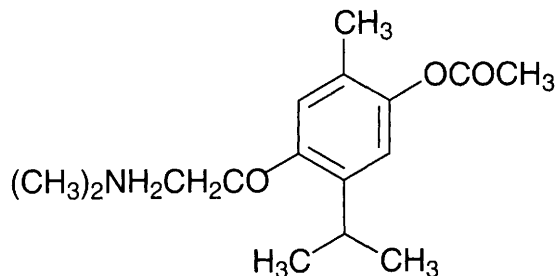
Reviews on human health effects, experimental toxicology, physico-chemical properties, ecotoxicology and workplace experience listed (13).

Adverse effects similar to phenol (9).

References

1. Heil, T. P. et al *J. Environ. Sci. Health, Part B* 1989, **B24**(4), 349-360.
2. *Osaka Shiritsu Daigaku Igaku Zasshi* 1956, **5**, 111.
3. *Food Cosmet. Toxicol.* 1964, **2**, 327.
4. Saunders, W. B. *Handbook of Toxicology* 1959, **5**, 172.
5. *Abderalden's Handbuch der Biologischen Arbeitsmethoden* 1935, **4**, 1289.
6. *J. Med. Chem.* 1980, **23**, 1350.
7. *Therapie* 1948, **3**, 109.
8. Kar, A. B. et al *J. Sci. Ind. Res. Sect. C: Biol. Res.* 1960, **19**, 264-267.
9. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
10. Smeenk, G. et al *Br. J. Dermatol.* 1987, **116**, 223-231.
11. Fukuda, S. *Shigaku* 1987, **74**(6), 1365-1384 (Japan.) (*Chem. Abstr.* **107**, 823y).
12. Arai, T. *Shigaku* 1988, **76**(1), 24-35 (Japan.) (*Chem. Abstr.* **109**, 204494t).
13. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T155 thymoxamine



$C_{16}H_{25}NO_3$

Mol. Wt. 279.38

CAS Registry No. 54-32-0

Synonyms phenol, 4-[2-(dimethylamino)ethoxy]-2-methyl-5-(1-methylethyl)-, acetate (ester); carvacrol, 5-[2-(dimethylamino)ethoxy]-, acetate (ester); Arlytene; Moxisylyte; Opilon; Sympal; Vasolklin
Uses Peripheral vasodilator. Adrenergic blocker.

Physical properties

M. Pt. 208-210°C

Mammalian & avian toxicity

Metabolism and toxicokinetics

Metabolised in rats and humans to the sulfate conjugates of desacetylthymoxamine and *N*-monodesmethyldesacetylthymoxamine and excreted in urine and faeces (1)

Other effects

Other adverse effects (human)

Hydrochloride may cause nausea, diarrhoea, vertigo and flushing of the skin. Overdosage may cause hypotension (2).

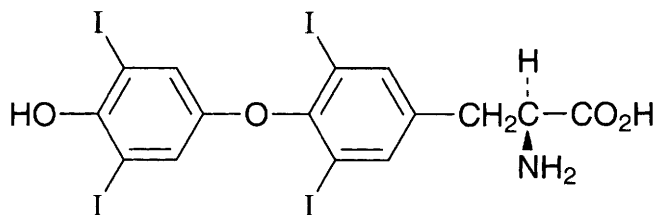
Any other adverse effects

Perfusion of the anterior chamber of adult pigmented rabbits with 1 ml of 0.02% or 0.2% thymoxamine hydrochloride caused no effects with 0.02%, but corneal swelling and reduction of intra-ocular pressure on day 1 with 0.2% (3).

References

1. Duchene, P. et al *Xenobiotica* 1988, 18(8), 919-928.
2. Martindale: *The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
3. Green, K. et al *Lens Eye Toxic. Res.* 1990, 7(3), 121-132

T156 L-thyroxine



$C_{15}H_{11}I_4NO_4$

Mol. Wt. 776.87

CAS Registry No. 51-48-9

Synonyms *o*-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-L-tyrosine; Levothyroxine; 3,3',5,5'-tetraiodothyronine; Thyroideum; T_4 (hormone); Thyroxinal

EINECS No. 200-101-1

RTECS No. YP 2833500

Uses Thyroid hormone.

Occurrence An amino acid of the thyroid gland.

Physical properties

M. Pt. 235-236°C (decomp.)

Solubility Water: 15 mg 100 ml⁻¹ (sodium salt) at 25°C. Organic solvents: ethanol

Ecotoxicity

Toxicity to other species

In late pre- to pro-metamorphic *Rana catesbeiana* injected with ¹²⁵I-thyroxine, the highest uptake of label occurred in the pineal followed by intestine, ventral skin, and pituitary, the lowest in thyroid and brain, and intermediate in hindlimb, tail, and gills (1).

Mammalian & avian toxicity

Acute data

TD_{Lo} oral man, woman 63, 400 µg l⁻¹, respectively (2,3).

LD₅₀ intraperitoneal, subcutaneous rat 20, 50 mg kg⁻¹, respectively (sodium salt) (4).

Sub-acute and sub-chronic data

Rats administered 500 µg day⁻¹ for 2 days showed marked stimulation of the proliferative activity in the epithelium of the pancreatic acini. The mean 24-hourly mitotic index was increased 15×, and the number of cells synthesising DNA was increased >20× compared with controls (5).

Metabolism and toxicokinetics

Plasma t_{1/2} 6-7 days in humans (6).

Other effects

Other adverse effects (human)

Adverse effects of administration of the sodium salt are symptoms of hyperthyroidism, including tachycardia, excitability, heat intolerance, and gastrointestinal disturbances (6).

A child aged 2 months ingested several tablets containing 0.15 mg of the sodium salt. The only symptoms were mild hypertension and tachycardia (7).

Any other adverse effects

It was previously thought that administration of thyroxine in mid-gestation could prevent spontaneous cleft lip in foetuses of genetically predisposed mice, but a study of mice given 0-0.2 mg mouse⁻¹ on days 10-12 of gestation showed increased mortality of cleft lip embryos compared with controls (8).

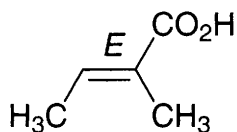
Other comments

D-Isomer used as antihyperlipoproteinemic.

References

1. Wright, M. L. et al *Comp. Biochem. Physiol., Part A: Mol. Integr. Physiol.* 1997, **118A**(3), 691-698.
2. *J. Toxicol.* 1983, **20**, 517.
3. *Intensive Care Med.* 1987, **13**, 33.
4. *Drugs in Japan. Ethical Drugs* 6th ed., 1982, 905, Yakugyo Jiho Co., Tokyo, Japan.
5. Markelova, I. V. et al *Bull. Exp. Biol. Med.* 1971, **72**, 942-944.
6. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
7. Roesch, C. et al *Ann. Emerg. Med.* 1985, **14**, 1114-1115.
8. Juriloff, D. M. *Dev. Pharmacol. Ther.* 1981, **2**, 17-31

T157 tiglic acid



C₅H₈O₂

Mol. Wt. 100.12

CAS Registry No. 80-59-1

Synonyms (E)-2-methyl-2-butenic acid; (E)-2-methylcrotonic acid; (E)-2,3-dimethylacrylic acid; trans-α,β-dimethylacrylic acid; (E)-α-methylcrotonic acid; trans-2-methylcrotonic acid

EINECS No. 201-295-0

RTECS No. GQ 5430000

Uses The esters in perfumes and flavouring agents; breaker of emulsions.

Occurrence Found in croton oil as glyceride, as butyl ester in oil of the Roman camomile and as geranyl tiglate in oil of geranium. Formed during charcoaling of maple wood.

Physical properties

M. Pt. 63.5-64°C **B. Pt.** 198.5°C **Specific gravity** 0.972

Solubility Water: sparingly soluble in cold water, freely soluble in hot water. Organic solvents: ethanol, diethyl ether

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird 111 mg kg⁻¹ (1).

Irritancy

Dermal rabbit (24 hr) 500 mg caused severe irritation (2).

Other comments

Vesicant.

References

1. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
2. *Food Chem. Toxicol.* 1982, **20**, 837

Sn

Sn

Mol. Wt. 118.71

CAS Registry No. 7440-31-5

Synonyms C.I. 77860; C.I. pigment metal 5; metallic tin; tin flake; tin powder; silver matt powder

EINECS No. 231-141-8

RTECS No. XP 7320000

Uses Used for tin plating and in soldering alloys, babbitt and type metals. In manufacture of tin salts, collapsible tubes.

Occurrence Occurs in minerals cassiterite, stannite and tealite. Forms $6 \times 10^{-4}\%$ of Earth's crust. Detected in soils, usually $<200 \text{ mg kg}^{-1}$ (1).

Physical propertiesM. Pt. 231.9°C B. Pt. 2507°C Specific gravity 7.31 Volatility v.p. 1 mmHg at 1492°C **Occupational exposure**US-TWA 2 mg m^{-3} **Ecotoxicity****Fish toxicity**LC₅₀ (28 day) rainbow trout 0.42 mg l^{-1} (form unspecified) (2).**Invertebrate toxicity**LC₅₀ (48 hr) *Daphnia magna* 42 mg l^{-1} (form unspecified) (3).EC₅₀ (21 day) *Daphnia magna* 1.5 mg l^{-1} (form unspecified) (3).LC₅₀ (144 hr) *Gammarus lacustris* 10 mg l^{-1} (form unspecified) (4).LC₅₀ (192 hr) *Gammarus pulex* 10 mg l^{-1} (form unspecified) (4).**Bioaccumulation**

Escherichia coli, *Sphaerotilus* sp. and *Saccharomyces cerevisiae* were able to absorb tin to a maximum of $<1.0 \text{ g metal g organism}^{-1}$ (form unspecified) (5).

Present in seawater up to $3 \text{ } \mu\text{g l}^{-1}$ but reports of occurrence in marine organisms are rare, although accumulation by the sponge *Terpius zeteki* has been reported (1,6).

Environmental fate**Nitrification inhibition**

$50 \text{ } \mu\text{g ml}^{-1}$ (as stannous chloride) inhibited nitrogenase activity by $\sim 70\%$ (7).

Mammalian & avian toxicity**Sub-acute and sub-chronic data**

Intratracheal administration of 50 mg of metallic tin dust to rats was well tolerated and did not produce fibrosis within 1 yr (8).

Metabolism and toxicokinetics

Inorganic tin is poorly absorbed from the gastro-intestinal tract ($<5\%$) (9,10).

Highest concentrations after oral and parenteral administration (form unspecified) were found in the kidney, liver and bone (9,10).

The main route of excretion of inorganic tin is via the kidney although a small amount is excreted in bile (10).

Rarely detected in the tissues of stillborn infants indicating it does not readily cross the placental barrier (11).

It was observed that rats absorbed a single dose of tin(II) more efficiently than tin(IV) ($2.85 \text{ vs. } 0.64\%$) (10).

Eight human subjects excreted 4 × as much tin (122 vs. 29 µg Sn day⁻¹) when fed 50 mg rather than 0.11 mg Sn day⁻¹ (12).

It has been found in at least trace amounts in most mammalian tissues (11).

In rats found to be accumulated in tibias, kidneys and livers in proportion to dietary intake (13).

Genotoxicity

In vitro tin(II) was readily taken up by ovary cells and damaged the DNA in the cells (14).

Other effects

Other adverse effects (human)

Ingestion of a fruit punch stored in a tin can, containing a tin concentration of 2000 mg l⁻¹, resulted in acute gastroenteritis. The initial symptoms were bloatedness, nausea, stomach cramps, vomiting and mild diarrhoea (15).

Other, similar outbreaks have been reported (1,15-17).

Individuals have developed symptoms, including nausea, abdominal cramping, diarrhoea and vomiting, after consuming canned juices or acidic punches prepared in tinned vessels (13).

Ingestion of tin reduced the calcium content of bone and serum, and increased kidney calcium levels (14,18,19).

Any other adverse effects

Ingestion of tin has been demonstrated to depress serum alkaline phosphatase and serum lactic dehydrogenase (20).

Animals injected with tin had decreased activity of γ-aminolevulinic dehydratase (21).

Growth of rats was depressed when dietary levels were elevated above 500 µg g⁻¹ (22).

Collagen synthesis was depressed in bones of rats treated orally with tin (23).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (24).

Other comments

Reviews on human health effects, experimental toxicology, environmental effects, ecotoxicology, exposure levels, epidemiology and workplace experience listed (25).

References

1. IPCS Environmental Health Criteria No. 15, 1980, WHO, Geneva, Switzerland.
2. Birge, W. J. et al *Aquatic Toxicity Testing on Inorganic Elements Occurring in Oilshale* EPA 600/9-80-022, 1980, Natl. Tech. Inf. Ser., Springfield, VA, USA.
3. Biesinger, K. E. et al *J. Fish Res. Board Can.* 1972, **29**, 1691-1700.
4. Zencirci, N. *Hydrobiologica* 1980, **69**, 179-186.
5. Zhu, H. *Shanghai Huanjing Kexue* 1988, **7**(5), 33-35.
6. Bowen, V. T. et al *J. Mar. Res.* 1951, **10**, 153-167.
7. Dubey, S. K. et al *Biol. Met.* 1989, **2**, 55-60.
8. Robertson, A. J. *Symposium on Industrial Pulmonary Diseases* 1960, 168-184, Little-Brown, Boston, USA.
9. Furchner, J. E. et al *Health Phys.* 1976, **31**, 219-224.
10. Hiles, R. A. *Toxicol. Appl. Pharmacol.* 1974, **27**, 366-379.
11. Schroeder, H. A. et al *Tin J. Chron. Dis.* 1964, **17**, 483-502.
12. Johnson, M. A. et al *Am. J. Clin. Nutr.* 1982, **35**, 655-660.
13. Greger, J. L. et al *Nutr. Toxicol.* 1987, **2**, 223-247.
14. McLean, J. R. N. et al *Mutat. Res.* 1983, **119**, 195-201.
15. Warburton, S. et al *Public Health Res. (Wash.)* 1962, **77**, 798-800.
16. Nehring, P. *Ind. Obst Gemueseverwert.* 1972, **57**, 489-492 (Ger.).
17. Svensson, V. *Hyg. Och. Miljoe* 1975, (6), 25-27.
18. Yamaguchi, M. et al *Toxicol. Lett.* 1981, **9**, 207-209.

19. Yamamoto, T. et al *J. Toxicol. Environ. Health* 1976, **1**, 749-756.
20. Yamaguchi, M. et al *Toxicology* 1980, **16**, 267-273.
21. Johnson, M. A. et al *J. Nutr.* 1985, **115**, 615-624.
22. de Groot, A. P. *Food Cosmet. Toxicol.* 1973, **11**, 955-962.
23. Ogoshi, K. et al *Toxicol. Appl. Pharmacol.* 1981, **58**, 331-332.
24. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
25. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T159 tin(II) chloride



Cl_2Sn Mol. Wt. 189.62 CAS Registry No. 7772-99-8

Synonyms C.I. 77864; dichlorotin; stannous dichloride; tin dichloride; Uniston CR-HT 200

EINECS No. 231-868-0

RTECS No. XP 8700000

Uses Reducing agent. Used in tinning by galvanic methods, in liquor finishing of wire and in sensitising of glass and plastic before metallising. A mordant in dyeing with cochineal. Tanning agent. Stain remover. Catalyst. Analytical reagent. In manufacture of pharmaceuticals, tin chemicals, colour pigments, sensitised paper, lubricating oils additives.

Physical properties

M. Pt. 37-38°C B. Pt. 247°C Specific gravity 3.95

Solubility Water: soluble. Organic solvents: acetone, diethyl ether, ethanol, isobutyl alcohol, methyl acetate, methyl ethyl ketone

Occupational exposure

DE-MAK 2 mg m⁻³ (as Sn) (inhalable dust fraction)

UK-LTEL 2 mg m⁻³ (as Sn)

UK-STEL 4 mg m⁻³ (as Sn)

US-TWA 2 mg m⁻³ (as Sn)

Ecotoxicity

Invertebrate toxicity

LC₅₀ (1 day, 2 day) *Daphnia magna* 37, 19.5 mg l⁻¹, respectively (1).

EC₅₀ (2 day, 4 day) *Crangonyx pseudogracilis* 71.8, 50.1 mg l⁻¹, respectively (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, rabbit, mouse, 700, 1000, 1200 mg kg⁻¹, respectively (3,4).

LD_{Lo} subcutaneous dog, guinea pig 159, 400 mg kg⁻¹, respectively (5,6).

LD₅₀ intravenous mouse 17.8 mg kg⁻¹ (7).

LD₅₀ intraperitoneal mouse 105 mg kg⁻¹ (8).

Sub-acute and sub-chronic data

Wistar rats given 3 or 10 g kg⁻¹ in diet for 4 wk developed slight anaemia, retarded growth and reduced food intake, and oedema and atrophy of the pancreas (9).

Carcinogenicity and chronic effects

National Toxicology Program tested rats and mice via feed. No evidence for carcinogenicity in ♀ rats and ♂, ♀ mice, equivocal evidence for carcinogenicity in ♂ rats (10).

Rats and mice administered 5 mg l⁻¹ in drinking water for life did not have an increased incidence of tumours compared with controls (11).

Rats exposed to 5 mg l⁻¹ in drinking water for life had vacuolar changes in the renal tubules of ♂ and fatty degeneration of the liver in ♂ (12).

Teratogenicity and reproductive effects

Administration of 0, 20, 100 or 500 mg kg⁻¹ to pregnant rats orally on days 7-12 gestation resulted in teratogenic effects on the early growing embryo and protruding tongue of the foetus. Some tin chloride was retained by the placenta, but some was diverted to the foetus (13).

Rats fed 10 g kg⁻¹ in diet for 13 wk suffered testicular damage (9).

Metabolism and toxicokinetics

<50% absorbed from the gastro-intestinal tract, with highest concentrations in the kidney, liver and bone.

Oxidation during absorption and systemic transportation is unlikely (14-16).

The major route of excretion in rats is via the kidney, although some may be excreted in bile (14).

Irritancy

Application of 1% solution to the abraded skin of rabbits caused intradermal pustule formation and epidermal destruction. There was no effect on intact skin. Soluble tin salts are gastric irritants (9).

Genotoxicity

Escherichia coli SOS Chromotest with and without metabolic activation positive (17).

In vitro Chinese hamster ovary cells with and without metabolic activation sister chromatid exchanges positive, chromosomal aberrations negative (18).

Other effects

Any other adverse effects

Rats administered tin(II) chloride dihydrate single dose ~LD₅₀ produced ataxia, muscular weakness and central nervous system depression (19).

A single subcutaneous injection of 5.6-56.4 mg kg⁻¹ to rat liver increased haem oxygenase activity three-fold after 16 hr (20).

A single intraperitoneal injection of 44.4 mg kg⁻¹ to rats caused extensive necrosis of kidney epithelial cells, mainly involving the proximal tubules (21).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Chlorides: guide level 25 mg l⁻¹ (22).

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (23).

References

1. Khangarot, B. S. et al *Acta Hydrochim. Hydrobiol.* 1987, **15**, 427.
2. Martin, T. R. et al *Water Res.* 1986, **20**(9), 1137-1147.
3. *Food and Agricultural Organisation of United Nations Report* 1970, **48A**, 75, FAO-United Nations, Washington, DC, USA.
4. *Food Res.* 1942, **7**, 313.
5. *Environ. Qual. Saf. Suppl.* 1975, **1**, 1.
6. *Br. Med. J.* 1913, **2**, 217.
7. Report NX 02202, US Army Armament Research and Development Command, Chemical Systems Laboratories, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD, USA.
8. *C. R. Hebd. Seances Acad. Sci.* 1963, **256**, 1043.
9. de Groot, A. P. et al *Food Cosmet. Toxicol.* 1973, **11**, 19-30.
10. *National Toxicology Program Research and Testing Division* 1992, Report No. PB 82242553, NIEHS, Research Triangle Park, NC, USA.

11. Kanisaiwa, M. et al *Cancer Res.* 1969, **29**, 892-895.
12. Schroeder, H. A. et al *J. Nutr.* 1968, **96**, 37-45.
13. Wu, Q. et al *Zhonghua Yufang Yixue Zazhi* 1990, **24**(1), 19-21 (Ch.) (*Chem. Abstr.* **113**, 54081).
14. Hiles, R. A. *Toxicol. Appl. Pharmacol.* 1974, **27**, 366-379.
15. Furchner, J. E. et al *Health Phys.* 1976, **31**, 219-224.
16. Kutzner, J. et al *Nucl. Med. (Stuttg.)* 1971, **10**, 286-297.
17. Olivier, P. et al *Mutat. Res.* 1987, **189**(3), 263-269.
18. Gulati, D. K. et al *Environ. Mol. Mutagen.* 1989, **13**(2), 133-193.
19. Conine, D. L. et al *Toxicol. Appl. Pharmacol.* 1975, **33**, 21-26.
20. Kappas, A. et al *Science* 1976, **192**, 60-62.
21. Yum, N. M. et al *Toxicol. Appl. Pharmacol.* 1976, **37**, 363-370.
22. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
23. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T160 tin(IV) chloride



Cl₄Sn

Mol. Wt. 260.52

CAS Registry No. 7646-78-8

Synonyms tetrachlorostannane; Libavium fuming spirit; stannic chloride; stannic tetrachloride; tetrachlorotin; tin tetrachloride

EINECS No. 231-588-9

RTECS No. XP 8750000

Uses Used as a mordant. For reviving colours and as a stabiliser for soap colours and perfumes. As dehydrating agent in organic synthesis. In ceramics to produce abrasion-resistant or light-reflecting coatings.

Physical properties

M. Pt. -33°C B. Pt. 114°C Specific gravity 2.26 Volatility v.p. 10 mmHg at 10°C

Solubility Organic solvents: acetone, benzene, carbon tetrachloride, ethanol, gasoline, kerosene, toluene

Occupational exposure

DE-MAK 2 mg m⁻³ (as Sn) (inhalable dust fraction)

UK-LTEL 2 mg m⁻³ (as Sn)

UK-STEL 4 mg m⁻³ (as Sn)

US-TWA 2 mg m⁻³ (as Sn)

UN No. 1827 (anhydrous); 2440 (pentahydrate) HAZCHEM Code 4WE (anhydrous); 2X (pentahydrate)

Conveyance classification corrosive substance

Supply classification corrosive

Risk phrases Causes burns – Irritating to the respiratory system (R34, R37)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep container tightly closed and dry – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S7/8, S26, S45)

Environmental fate

Carbonaceous inhibition

Almost complete inhibition of methanogenic bacteria *Methanococcus thermolithotrophicus*, *Methanococcus deltae* ΔLH and *Methanobarkeri* 227 occurred with 260.5 mg l⁻¹ (1).

Mammalian & avian toxicity

Acute data

LC₅₀ (10 min) inhalation rat 2300 mg mg⁻³ (2).

LD₅₀ intraperitoneal mouse 101 mg kg⁻¹ (3).

Metabolism and toxicokinetics

Inorganic tin is poorly absorbed from the gastro-intestinal tract (<5%) and mainly excreted through the kidneys (4-6).

Irritancy

Guinea pigs exposed to 3 mg l⁻¹ for 10 min day⁻¹ for several months had only transient irritation of the nose and eyes (7).

Soluble tin salts are gastric irritants (8).

Sensitisation

34/95 subjects patch tested for sensitivity with 1% solution developed erythema, 14/95 developed erythema and oedema and 1/95 developed erythema, oedema, and papules (9).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA102, TA1537, TA2637 negative (metabolic activation unspecified) (10).

Salmonella typhimurium TA1537, TA2637 in the presence of 9-aminoacridine hydrochloride (9-AA) positive, giving a stronger response than 9-AA alone (10).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Chlorides: guide level 25 mg l⁻¹ (11).

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (12).

Other comments

Reviews on human health effects, experimental toxicology, ecotoxicology and physico-chemical properties listed (13).

References

1. Boopathy, R. et al *Appl. Environ. Microbiol.* 1991, **57**(4), 1189-1193.
2. *Toxicologist* 1981, **1**, 77.
3. C. R. *Hebd. Seances Acad. Sci.* 1963, **256**, 1043.
4. Hiles, R. A. *Toxicol. Appl. Pharmacol.* 1974, **27**, 366-379.
5. Kutzner, J. et al *Nucl. Med. (Stuttg.)* 1971, **10**, 286-297.
6. Furschner, J. E. et al *Health Phys.* 1976, **31**, 219-224.
7. Pedley, F. G. *J. Ind. Hyg.* 1927, **9**, 43-47.
8. de Groot, A. P. et al *Food Cosmet. Toxicol.* 1973, **11**, 19-30.
9. Namikoshi, T. et al *J. Oral Rehabil.* 1990, **17**(4), 377-381.
10. Ogawa, H. I. et al *Jpn. J. Genet.* 1987, **62**, 159-162.
11. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
12. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
13. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T161 tin(II) fluoride



F₂Sn

Mol. Wt. 156.71

CAS Registry No. 7783-47-3

Synonyms tin difluoride; tin bifluoride; Fluoristan; stannous fluoride

EINECS No. 231-999-3

RTECS No. XQ 3450000

Uses As an anticaries ingredient in dentifrices.

Physical properties

M. Pt. 213°C **B. Pt.** 850°C **Specific gravity** 4.570 at 25°C

Solubility Water: ~300 g l⁻¹. Organic solvents: practically insoluble in chloroform, diethyl ether, ethanol

Occupational exposure

UK-LTEL 2 mg m⁻³ (as Sn)

UK-STEL 4 mg m⁻³ (as Sn)

US-TWA 2 mg m⁻³ (as Sn)

Ecotoxicity

Invertebrate toxicity

Tin difluoride dramatically alters the growth and metabolism of *Streptococcus mutans*. The antibacterial action is associated with a large uptake of Sn into the bacterial cells (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral Swiss white mouse 25.5-31.2 mg kg⁻¹ (as F) (2,3).

LD₅₀ oral rat 45.7 mg kg⁻¹ (as F) (3).

Sub-acute and sub-chronic data

Single intraperitoneal injections of 0.5 mmol kg⁻¹ F⁻ and repeated intraperitoneal injections of 0.25 mmol kg⁻¹ F⁻ (as NaF or SnF₂) to ♂ rats showed both compounds to produce early lesions of kidney tubule. Disturbance of kidney function with an increase of diuresis and phosphaturia and a decrease of natriuria and kaliuria were more marked in SnF₂-treated animals, as was the decrease of urine γ-glutamyl transferase after a few days, showing that Sn nephrotoxicity adds to that of F⁻ and antagonises tubule regeneration (4).

Carcinogenicity and chronic effects

Inadequate evidence for carcinogenicity of inorganic fluorides used in drinking water to humans, inadequate evidence for carcinogenicity to animals, IARC classification group 3 (5).

Teratogenicity and reproductive effects

Intraperitoneal injections of ≥10 mg kg⁻¹ caused varying degrees of embryoletality and teratogenicity in small groups of mice (6).

Metabolism and toxicokinetics

Fluoride ion is rapidly absorbed from the gut (7).

Genotoxicity

Salmonella typhimurium microsomal mutagenicity assay positive (4 μmol plate⁻¹) (8).

Bacillus subtilis rec assay system weakly positive (9).

Other effects

Other adverse effects (human)

The immediate effects of the ingestion of a toxic dose of soluble inorganic fluoride include vomiting, abdominal pain and diarrhoea (10).

Any other adverse effects

Accumulation of cAMP in isolated rat thoracic aorta and diaphragm is stimulated by SnF₂. A significant increase was produced by 0.01 µM SnF₂ (11).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Fluoride: maximum admissible concentration 1500 µg l⁻¹ (8-12°C), 700 µg l⁻¹ (25-30°C). Maximum admissible concentration varies according to average temperature in geographical area concerned (12).

Recognised by the US Food and Drug Administration as safe and effective in topical anticaries products at 0.4% in dentifrices and anhydrous glycerine gels and in a stable form for mixing with water to produce a dental rinse containing 0.1% tin difluoride (13).

In the EC the concentration of total fluorine in oral hygiene products is limited to a maximum of 0.15% (14).

Other comments

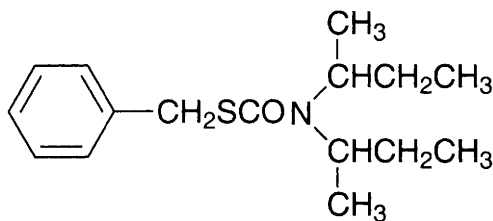
Forms an oxyfluoride, SnOF₂, on exposure to air.

Aqueous solutions decompose within a few hours, with the formation of a white precipitate; they slowly attack glass (15).

References

1. Camosci, D. A. et al *J. Dent. Res.* 1984, **63**(9), 1121-1125.
2. Segreto, V. A. et al *J. Dent. Res.* 1961, **40**, 623.
3. Lim, J. K. et al *Caries Res.* 1978, **12**, 177-179.
4. Kessabi, M. et al *Toxicol. Lett.* 1981, **7**(6), 463-467.
5. IARC Monograph 1987, **Suppl.** 7, 63.
6. Stratmann, K.-R. *Dtsch. Zahnärztl. Z.* 1979 **34**, 484-486.
7. Cremer, H.-D. et al *Fluorides and Human Health* 1970, pp. 75-91, WHO, Geneva, Switzerland.
8. *Mutat. Res.* 1981, **90**, 91.
9. Kanematsu, N. et al *Shika Kiso Igakkai Zasshi* 1985, **27**(1), 372-374.
10. Hodge, H. C. et al *Fluorine Chemistry* Vol. 4, 1972, pp. 113-119, Academic Press, New York, NY, USA.
11. Allman, D. W. et al *Res. Commun. Chem. Pathol. Pharmacol.* 1986, **52**(3), 275-284.
12. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
13. *Fed. Regist.* 1980, **45**(144), 49450.
14. *Off. J. Eur. Communities* 1976, **19A**, 30.
15. *Martindale. The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK

T162 tiocarbazil



C₁₆H₂₅NOS

Mol. Wt. 279.45

CAS Registry No. 36756-79-3

Synonyms carbamothioic acid, bis(1-methylpropyl)-S-(phenylmethyl) ester; Drepamon; M3432; tiocarbazil

EINECS No. 253-190-4

RTECS No. EZ 3970000

Uses Herbicide.

Physical properties

B. Pt. 130-132°C at 0.1 mmHg **Specific gravity** 1.023 at 20°C **Partition coefficient** log P_{ow} 4.40 (1)

Volatility v.p. 7.0×10^{-4} mmHg at 50°C

Solubility Water: 2.5 mg l⁻¹ at 30°C. Organic solvents: miscible with polar and non-polar organic solvents

Ecotoxicity

Fish toxicity

LC₅₀ fish (species and duration unspecified) ≥8 mg l⁻¹ (1).

Invertebrate toxicity

LC₅₀ (duration unspecified) *Australorbis glabratus* >60 mg l⁻¹ (1).

Not hazardous for honeybees (2).

Environmental fate

Abiotic removal

Stable to hydrolysis at pH 5.6-8.4, slightly decomposed at >30 days at 40°C in aqueous ethanol at pH 1.5 (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral chicken, pheasant, quail >10,000 mg kg⁻¹ (1).

LD₅₀ oral rat, rabbit, guinea pig >10,000 mg kg⁻¹ (1).

LD₅₀ oral mouse 8000 mg kg⁻¹ (1).

LD₅₀ dermal rat, rabbit >1200 mg kg⁻¹ (1).

Carcinogenicity and chronic effects

In 2-yr feeding trials, rats and dogs receiving 1000 mg kg⁻¹ suffered no ill-effects except slight weight loss in ♂ dogs (1).

Rats receiving 300 mg kg⁻¹ for three generations showed no ill-effects (1).

Metabolism and toxicokinetics

Oral administration 1 g kg⁻¹ of tiocarbazil to animals is almost totally eliminated, by seven days after treatment, unchanged in the faeces and as metabolites in the urine. Minimum concentration of tiocarbazil and its metabolites have been found in the blood and main organs 48 hr after administration (2).

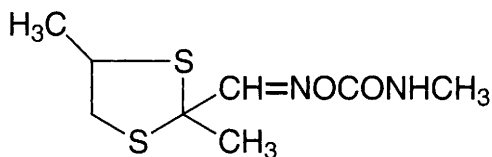
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (3).
Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (4).
The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (5).
WHO Toxicity Class Table 5 (6).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
4. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
5. 1967 *Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
6. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21

T163 tirpate



$\text{C}_8\text{H}_{14}\text{N}_2\text{O}_2\text{S}_2$

Mol. Wt. 234.34

CAS Registry No. 26419-73-8

Synonyms 2,4-dimethyl-1,3-dithiolane-2-carboxaldehyde *o*-[(methylamino)carbonyl]oxime;

2,4-dimethyl-1,3-dithiolane-2-carboxyaldehyde *o*-(methylcarbamoyl)oxime

Uses Nematicide.

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1 mg kg⁻¹ (1).

LD₅₀ dermal rat 300 mg kg⁻¹ (2).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (3).
Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (4).

References

1. *World Rev. Pest Control* 1970, 9, 119.
2. *Guide to Chemicals used in Crop Protection* 1973, 6, 213, Information Canada, Ottawa, Canada.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
4. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T164 titanium

Ti

Ti

Mol. Wt. 47.88

CAS Registry No. 7440-32-6

Synonyms Contimet 30; IMI 115; T60; Ti 160; VT 1-1

EINECS No. 231-142-3

RTECS No. XR 1700000

Uses As an alloy with copper and iron in titanium bronze. As addition to steel to add tensile strength. Added to aluminium to resist attack by salt solutions and organic acids. To remove traces of oxygen and nitrogen from incandescent lamps. Surgical aid in fracture fixation.

Occurrence Occurs as oxide in minerals rutile, ilmenite, perovskite, anatase, octahedrite, brookite. Also in minerals sphene, titanite and benitoite. Ninth most abundant element in the Earth's crust; 0.63% by weight.

Physical properties

M. Pt. 1677°C B. Pt. 3277°C Flash point 1200°C (solid metal), 250°C (powder)

Specific gravity 4.506 (α form) at 25°C, 4.400 (β form) at 2900°C

Occupational exposure

UN No. 2546 (dry); 1352 (wetted); 2878 (sponge granules or powder) HAZCHEM Code 4Y (dry); 1X (wetted); 4X (sponge granules) Conveyance classification spontaneously combustible substance (dry); flammable solid (wetted or sponge granules)

Ecotoxicity

Fish toxicity

LC₅₀ (28 day) rainbow trout 7.31 mg l⁻¹ (form unspecified) (1).

Bioaccumulation

Earthworms accumulated 16.3 mg kg⁻¹ dry weight after vermicomposting with wood chip bulking material for 6 months (undetected in worms prior to vermicomposting) (2).

Mammalian & avian toxicity

Carcinogenicity and chronic effects

Rats injected intramuscularly with fine titanium metal powder suspended in trioctanoin developed fibrosarcomas at the injection site and hepatomas and malignant lymphomas at the spleen (3).

Metabolism and toxicokinetics

Titanium as ⁴⁴Ti-oxalate was incubated with human blood and lung tissue. A low solubility in body fluids was observed, but there was a high affinity for lung and plasma proteins (4).

Other effects

Other adverse effects (human)

Several cases of malignant tumours have been reported associated with pacemakers which are covered in titanium, including scirrhomas mammary carcinomas, and adenocarcinoma, extramedullary plasmacytoma and malignant fibrosis histiocytoma (5-8).

Other comments

Physiologically indifferent metal causing no dysstasia, discomfort, pain, infection, bone resorption or psychological effects when used in implants (9).

Reviews on human health effects, experimental toxicology, environmental effects, ecotoxicology, exposure levels listed (10).

Toxicity reviewed (11).

References

1. Birge, W. J. et al *Aquatic Toxicity Tests on Inorganic Elements Occurring in Oil Shales* EPA 60/9-80-022, 1980, Natl. Tech. Inf. Serv., Springfield, VA, USA.
2. Harris, G. D. et al *Bio Cycle* 1990, **31**(1), 48-51.
3. Furst, A. *Geol. Soc. Am. Mem.* 1971, **123**, 109-130.
4. Edel, J. et al *Sci. Total. Environ.* 1990, **95**, 107-117.
5. Zafiracopoulos, P. et al *Lancet* 1974, **1**, 1114.
6. Magilligan, D. J. et al *PACE* 1980, **3**, 220-223.
7. Jamaker, W. R. et al *Ann. Thorac. Surg.* 1976, **21**, 354-356.
8. Fraedich, G. et al *Thorac. Cardiovasc. Surg.* 1984, **32**, 66-69.
9. Van Noort, R. J. *Mater. Sci.* 1987, **22**, 3801-3811.
10. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium.
11. Feigin, B. G. *Gig. Tr. Prof. Zabol.* 1988, (7), 30-33 (Russ.) (*Chem. Abstr.* **109**, 134136b)

T165 titanium dioxide



O₂Ti

Mol. Wt. 79.88

CAS Registry No. 13463-67-7

Synonyms C.I. 77891; C.I. Pigment White 6; TiOxide AD-M; Ti-Pure; titanium(IV) oxide; titanium peroxide; UV Titan; Tiona RCL-376; TiOxide; Hitox; Hombitan

EINECS No. 236-675-5

RTECS No. XR 2275000

Uses In titanium pigment manufacture. Food colour. Topical protectant. Rutile sand used for welding-rod coating materials, ceramic colorant and titanium source.

Occurrence Occurs as the minerals rutile, anatase, octahedrite, brookite, ilmenite and perovskite.

Physical properties

M. Pt. 1855°C (decomp.) **Specific gravity** 4.23 (rutile), 3.96 (anatase), 4.13 (brookite)

Solubility Water: Insoluble. Organic solvents: Insoluble

Occupational exposure

DE-MAK 1.5 mg m⁻³ (respirable fraction of aerosol)

FR-VME 10 mg m⁻³

SE-LEVL 5 mg m⁻³

UK-LTEL 10 mg m⁻³ (total inhalable dust); 4 mg m⁻³ (respirable dust)

US-TWA 10 mg m⁻³

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird, starling 100 mg kg⁻¹ (1).

Rats were administered 50 mg kg⁻¹ titanium dioxide dust intratracheally. The dust particles averaged 5 µm in diameter. Bronchoalveolar lavage was performed 24 hr later. Production of inducible nitric oxide synthase mRNA

increased. Alveolar neutrophil numbers increased, indicating an inflammatory response. Alveolar macrophage numbers decreased (2).

Carcinogenicity and chronic effects

National Toxicology Program investigated titanium dioxide in rats and mice. Designated non-carcinogen in rats and mice (3).

Rats were exposed to 0, 10, 50, 250 mg m⁻³ 6 hr day⁻¹, 5 day wk⁻¹ for 2 yr. Exposed groups had increased incidences of pneumonia, tracheitis, and rhinitis with squamous metaplasia in the anterior nasal cavity. At 50 and 250 mg m⁻³ rats showed a dose-dependent dust cell accumulation, a foamy macrophage response, Type II pneumocyte hyperplasia, alveolar proteinosis, alveolar bronchiolarisation, cholesterol granulomas, focal pleurisy and dust deposition in the tracheobronchial lymph nodes. No lung tumours were seen in rats at 10-50 mg m⁻³, but pulmonary lesions, bronchoalveolar adenomas and cystic keratinising squamous cell carcinomas occurred at 250 mg kg⁻¹ (4).

Irritancy

Dermal human (3 day) 300 µg caused mild irritation (5).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535 with and without metabolic activation negative (6).

In vitro Chinese hamster ovary cells with and without metabolic activation sister chromatid exchanges, chromosomal aberrations negative (7).

Drosophila melanogaster wing spot test negative (8).

In vitro rat liver epithelial cells, micronuclei negative (9).

Salmonella typhimurium, single cell gel (SCG) assay with mouse lymphoma L5178Y cells, mammalian cell mutation assay with L5178Y cells, chromosomal aberration assay with Chinese hamster CHL/IU cells negative or weakly positive in the absence of UV/visible light irradiation. SCG and chromosomal assays positive in the presence of UV/visible light irradiation (10).

Other effects

Other adverse effects (human)

Cancer incidence in employees exposed to titanium dioxide from 1956-1985 was compared with controls. A slightly increased incidence of cancer cases was observed in the exposed group, but analysis showed no increased risk of developing lung cancer compared with controls (11).

Legislation

Included in Schedule 4 (Release into Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (12).

Other comments

Anatase used for welding rod coatings, exterior house paints, acetate rayon, paper filling and coating, shoe whiteners and ceramics.

Reviews on human health effects, experimental toxicology, workplace experience, ecotoxicology, epidemiology and exposure levels listed (13).

Toxicity reviewed (14).

References

1. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
2. Blackford, J. A., Jr. et al *J. Toxicol. Environ. Health* 1997, **3**, 203-218.
3. *National Toxicology Program Research and Testing Division* 1992, Report No. PB2388780/AS, NIEHS, Research Triangle Park, NC, USA.
4. Lee, K. P. et al *Toxicol. Appl. Pharmacol.* 1985, **79**, 179-192.
5. Orill, V. A. et al *Cutaneous Toxicity* 1977, Academic Press, New York, NY, USA.
6. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-157.

7. Ivett, J. L. et al *Environ. Mol. Mutagen.* 1989, **14**(3), 165-187.
8. Tripathy, N. K. et al *Mutat. Res.* 1990, **242**(3), 169-180.
9. Linnainmaa, K. et al *Toxicol. In Vitro* 1997, **11**(4), 329-335.
10. Nakagawa, Y. et al *Mutat. Res.* 1997, **394**(1-3), 125-132.
11. Barckhaus, R. H. et al *Met. Ions Biol. Med. Proc. 1st. Symp.* 1st 1990, 284-288.
12. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
13. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
14. Feigin, B. G. *Gig. Tr. Prof. Zabol.* 1988, (7), 30-33 (Russ.) (*Chem. Abstr.* **109**, 134136b)

T166 titanium tetrachloride



Cl₄Ti

Mol. Wt. 189.69

CAS Registry No. 7550-45-0

Synonyms titanium chloride (TiCl₄) (T-4)-; tetrachlorotitanium; titanium(IV) chloride

EINECS No. 231-441-9

RTECS No. XR 1925000

Uses Manufacture of iridescent glass and artificial pearls. For producing smoke screen with ammonia. Formerly used as mordant in textile industry with potassium bitartrate.

Physical properties

M. Pt. -24.1°C **B. Pt.** 136.4°C **Specific gravity** 1.726

Solubility Water: soluble in cold water. Organic solvents: ethanol

Occupational exposure

UN No. 1838 **HAZCHEM Code** 4WE **Conveyance classification** corrosive substance

Supply classification corrosive

Risk phrases Reacts violently with water – Causes burns – Irritating to eyes and respiratory system (R14, R34, R36/37)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep container tightly closed and dry – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S7/8, S26, S45)

Mammalian & avian toxicity

Acute data

LC₅₀ (2 hr, 4 hr) inhalation mouse, rat 100, 460 mg m⁻³, respectively (1,2).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Chloride: guide level 25 mg l⁻¹ (3).

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (4).

Other comments

Toxicity reviewed (5).

References

1. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
2. *Toxicologist* 1981, 1, 76.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
4. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
5. Feigin, B. G. *Gig. Tr. Prof. Zabol.* 1988, (7), 30-33 (Russ.) (*Chem. Abstr.* 109, 134136b)

T167 titanium trichloride



Cl_3Ti

Mol. Wt. 154.24

CAS Registry No. 7705-07-9

Synonyms titanium chloride (TiCl_3); TAC 121; titanium(III) chloride; titanous chloride; trichlorotitanium

EINECS No. 231-728-9

RTECS No. XR 1924000

Uses Reducing agent. Used as an aqueous solution to estimate nitro-groups, ferric ions and per-salts. Stain remover in laundering.

Physical properties

M. Pt. 440°C (decomp.) **Specific gravity** 2.640 **Volatility** v.p. 10 mmHg at 21.3°C

Solubility Organic solvents: ethanol

Occupational exposure

UN No. 2441 (pyrophoric) **Conveyance classification** spontaneously combustible substance, corrosive

Mammalian & avian toxicity

Teratogenicity and reproductive effects

A single intratesticular injection of 12.3 mg kg⁻¹ caused total testicular necrosis in rats (1).

Legislation

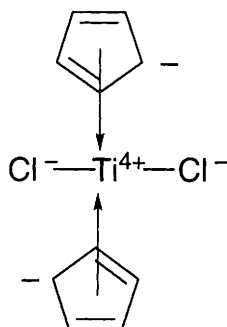
Limited under EC Directive on Drinking Water Quality 80/778/EEC. Chlorides: guide level 25 mg l⁻¹ (2).

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (3).

References

1. Kamboj, V. P. et al *J. Reprod. Fertil.* 1964, 7, 21-28.
2. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
3. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T168 titanocene dichloride



$C_{10}H_{10}Cl_2Ti$

Mol. Wt. 248.97

CAS Registry No. 1271-19-8

Synonyms dichlorobis(η^5 -2,4-cyclopentadien-1-yl)titanium; dichloride- π -cyclopentadienyltitanium; dichlorodicyclopentadienyltitanium; dichlorotitanocene; dicyclopentadienyldichlorotitanium

EINECS No. 215-035-9

RTECS No. XR 2050000

Uses Catalyst. With aluminium alkyls as Ziegler-Natta polymerisation catalyst.

Physical properties

M. Pt. $289 \pm 2^\circ C$ Specific gravity 1.60

Solubility Water: sparingly soluble. Organic solvents: benzene, carbon tetrachloride, chloroform, diethyl ether, ethanol, light petroleum, toluene

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat, mouse 25, 60 mg kg⁻¹, respectively (1,2).

LD₅₀ intravenous mouse 180 mg kg⁻¹ (3).

Carcinogenicity and chronic effects

National Toxicology Program tested rats via gavage. Equivocal evidence of carcinogenic activity (marginal increase in neoplasms which may be treatment related) in σ , \varnothing rats (4).

Teratogenicity and reproductive effects

Pregnant mice were administered 30 or 60 mg kg⁻¹ intraperitoneally as a single dose on days 8, 10, 12, 14 or 16 of gestation. 10% of foetuses at 30 mg kg⁻¹ and 40-50% at 60 mg kg⁻¹ had cleft palate on day 18 of gestation. A dose-dependent reduction in mean foetal body-weight after application on days 8-16 was also observed, as well as a decreased number of live foetuses per litter and a retardation of foetal ossification (5).

Metabolism and toxicokinetics

Following a single intraperitoneal injection of 60 mg kg⁻¹ to mice, 80-90 mg kg⁻¹ of titanium was accumulated in the liver and intestine after 24 and 48 hr, corresponding to liver:blood and intestine:blood ratios of 8-9. 10-15 mg kg⁻¹ was found in solid tumours growing subcutaneously on mice administered a single intraperitoneal dose after 24 and 96 hr (6).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (7).

In vitro mouse Balb/3T3 cells, Syrian hamster embryo cells, and Rauscher Murine leukaemia virus-infected Fischer 344 rat embryo cells without metabolic activation spontaneous neoplastic transformation positive (8).

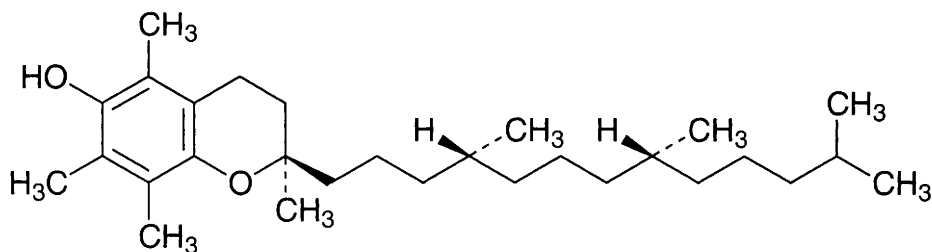
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC Chlorides: guide level 25 mg l⁻¹ (9).
Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (10).

References

1. *Progress Report for Contract No. PH-43-64-886* January 1965, Submitted to the National Cancer Institute by the Institute of Chemical Biology, University of San Francisco, CA, USA.
2. *Progress Report for Contract No. PH-43-64-886* August 1964, Submitted to the National Cancer Institute by the Institute of Chemical Biology, University of San Francisco, CA, USA.
3. *Report NX 00774*, US Army Research and Development Command, Chemical Systems Laboratory, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD, USA.
4. *National Toxicology Program Research and Testing Division* 1992, Report no. PB92-129576/AS, NIEHS, Research Triangle Park, NC, USA.
5. Koepf-Maier, P. et al *Toxicology* 1984, **33**, 171-181.
6. Koepf-Maier, P. et al *Toxicology* 1988, **51**(2-3), 291-298.
7. Haworth, S. et al *Environ. Mol. Mutagen.* 1983, **5**(Suppl. 1), 3.
8. Dunkel, V. C. et al *J. Natl. Cancer Inst.* 1981, **67**, 1303.
9. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
10. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T169 α -tocopherol



C₂₉H₅₀O₂

Mol. Wt. 430.71

CAS Registry No. 59-02-9

Synonyms (2*R*,4'*R*,8'*R*)- α -tocopherol; 2*H*-1-benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, [2*R*-[2*R**(4*R**,8*R**)]]-; vitamin E; antisterility vitamin; E306 (natural); E307 (synthetic)

EINECS No. 200-412-2

RTECS No. DJ 2900000

Uses Anti-oxidant. Antineoplastic agent. Dietary supplement.

Occurrence Widespread in foods. Richest sources are vegetable oils.

Physical properties

M. Pt. 2.5-3.5°C **B. Pt.** 200-220°C at 0.1 mmHg **Flash point** >110°C **Specific gravity** 0.950 at 25°C with respect to water at 4°C

Solubility Organic solvents: acetone, chloroform, diethyl ether, ethanol, fats, oils

Environmental fate

Abiotic removal

Slowly oxidised by atmospheric oxygen (1).

Mammalian & avian toxicity

Sub-acute and sub-chronic data

Intravenous newborn rabbit, 100 mg animals day⁻¹ for 6 or 7 days. Lipolysis was evident in the liver and spleen and indicated mild hepatotoxicity (2).

Metabolism and toxicokinetics

Absorption rat small intestine increased with increased bile salt concentration (3).

Enters the bloodstream via the chylomicrons in the lymph. It is widely distributed to all tissues and stored in adipose tissue. Some vitamin E is metabolised in the liver to glucuronides of tocopheronic acid and its γ -lactone. Eliminated in the urine and bile. Detected in human breast milk, but it is poorly transferred across the placenta (4).

Sensitisation

Contact dermatitis has been reported following skin contact in humans (4).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538 with and without metabolic activation negative (5).

In vitro Chinese hamster ovary cells, sister chromatid exchanges and chromosomal aberrations positive (metabolic activation unspecified) (6).

In vitro rat liver DNA damage positive (7).

Other effects

Other adverse effects (human)

Large doses may cause intestinal disturbances (4).

Has been reported to antagonise the effects of vitamin K, leading to an increase in blood clotting time in predisposed patients (4).

Other comments

Vitamin E appears to inhibit the development of lung tumourigenesis in mice treated with NNK, due partly to the regulation of polyamine metabolism (8).

Intraperitoneal σ mice 0.5 mg kg⁻¹ body weight lead acetate daily for 30 days caused a significant reduction in the activities of serum 3,3',5'-triiodothyronine and type I iodothyronine 5'-monodeiodinase and of antioxidant enzymes of the liver. Peroxidative reactions involving membrane components increased. Simultaneous administration of 5 mg kg⁻¹ vitamin E protected against all these effects (9).

Aids the supply of oxygen to heart and muscles. Essential in activity of red blood cells (2).

1 IU of vitamin E equals 1 mg *dl*- α -tocopherol acetate (4).

The human dietary requirement is 3 to 20 mg day⁻¹; the requirement increasing with increased dietary polyunsaturated fatty acids (4).

Deficiency is rare. In children with congenital disorders such as cystic fibrosis or biliary atresia, malabsorption of fat may lead to vitamin E deficiency. The major signs of deficiency are the development of myopathic and neurological disorders (4).

Inhibited the induction of stomach papillomas in rats, hamsters and mice, and skin tumours in mice (10,11).

Pretreatment of ϕ mice with α -tocopherol before administration of the mycotoxin zearalenone significantly inhibited DNA adduct formation in the liver (by 45%) and in the kidney (by 58%) (12).

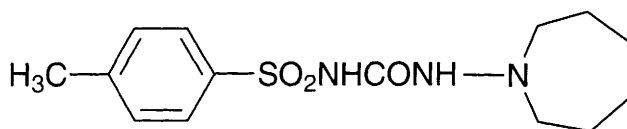
Largely destroyed by freezing (13).

References

1. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
2. Rivera, A. et al *Dev. Pharmacol. Ther.* 1990, **14**(4), 231-237.
3. Ueno, M. et al *Yukagaku* 1991, **40**(5), 400-405.
4. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
5. Prival, M. J. et al *Mutat. Res.* 1991, **260**, 321-329.

6. Rosenkranz, H. S. et al *Environ. Mol. Mutagen.* 1990, **16**, 149-177.
7. Russo, P. et al *Cancer Lett.* 1984, **25**, 163-170.
8. Kishimoto, M. et al *Cancer Lett. (Shannon, Irel.)* 1998, **126**(2), 173-178.
9. Chaurasia, S. S. et al *Toxicology* 1997, **124**(3), 203-210.
10. Ito, N. et al *Shokuhin Eisei Kenkyu* 1990, **40**(3), 7-18, (Japan.) (*Chem. Abstr.* **113**, 96278x).
11. Perchellet, J. P. et al *Cancer Res.* 1987, **47**(2), 477-485.
12. Grosse, Y. et al *Cancer Lett. (Shannon Irel.)* 1997, **114**(1-2), 225-229.
13. Hanssen, M. et al *E for Additives* 1987, 157, Thorsons, Wellingborough, UK

T170 tolazamide



$C_{14}H_{21}N_3O_3S$

Mol. Wt. 311.41

CAS Registry No. 1156-19-0

Synonyms N-[[[(hexahydro-1H-azepin-1-yl)amino]carbonyl]-4-methylbenzenesulfonamide; 1-(hexahydro-1H-azepin-1-yl)-3-(p-tolysulfonyl)urea; Norglycin; tolanase; tolinase; U17835

EINECS No. 214-588-3

RTECS No. YT 4400000

Uses Oral hypoglycaemic agent.

Physical properties

M. Pt. 170-173°C

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 1000 mg kg⁻¹ (1).

LD₅₀ intraperitoneal mouse 1000 mg kg⁻¹ (1).

Carcinogenicity and chronic effects

National Toxicology Program tested tolazamide in mice and rats in feed. Designated non-carcinogen in mice and rats (2).

Metabolism and toxicokinetics

Absorbed from the gastro-intestinal tract in humans and bound to plasma proteins, $t_{1/2}$ 7 hr. Metabolised in the liver and excreted in urine, mainly as metabolites (unspecified) (3).

Irritancy

Skin rashes and pruritus may occur in humans (3).

Genotoxicity

Salmonella typhimurium TA100, TA1535 with and without metabolic activation negative (4).

Other effects

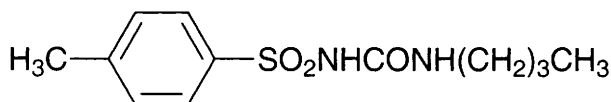
Other adverse effects (human)

Adverse effects include gastro-intestinal disturbances, increased appetite and weight gain, hypoglycaemia, hypersensitivity reactions and abnormal secretion of antidiuretic hormone (5).

References

1. *J. Med. Chem.* 1981, **24**, 1521.
2. *National Toxicology Program Research and Testing Division* 1992, Report No. PB 284610/AS, NIEHS, Research Triangle Park, NC, USA.
3. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
4. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-157.
5. Paice, B. J. et al *Adv. Drug React. Acute Poisoning Rev.* 1985, **4**, 23-36

T171 tolbutamide



C₁₂H₁₈N₂O₃S

Mol. Wt. 270.35

CAS Registry No. 64-77-7

Synonyms N-[(butylamino)carbonyl]-4-methylbenzenesulfonamide; 1-butyl-3-(p-tolylsulfonyl)urea; Artosin; Butamide; Diabetol; Oralin; Willbutamide

EINECS No. 200-594-3

Uses Antidiabetic. Veterinary hypoglycaemic agent.

Physical properties

M. Pt. 128.5-129.5°C

Solubility Organic solvents: acetone, chloroform, diethyl ether, ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 490, 2490 mg kg⁻¹, respectively (1,2).

LD₅₀ subcutaneous mouse 980 mg kg⁻¹ (3).

LD₅₀ intraperitoneal mouse, rat 700, 860 mg kg⁻¹, respectively (4,5).

LD₅₀ intravenous rat, mouse 700, 770 mg kg⁻¹, respectively (6).

Carcinogenicity and chronic effects

National Toxicology Program investigated tolbutamide in rats and mice via feed. Designated non-carcinogen in both species (7).

Metabolism and toxicokinetics

A single dose of 1 g 70 kg⁻¹ administered to 31 non-smoking ♂ was excreted, in varying amounts, in 24 hr as hydroxy- and carboxy-tolbutamide (8).

Readily absorbed from the gastro-intestinal tract and bound to plasma proteins; t_{1/2} 4-8 hr. Metabolised in the liver and excreted in urine, mainly as metabolites. Has been detected in breast milk (9).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538 with and without metabolic activation negative (10).

In vivo Chinese hamster, mouse bone marrow cells sister chromatid exchanges positive, chromosomal aberrations negative (10).

In vivo C3H and C57Bl mice micronucleus test positive and negative, respectively (10).

In vivo Chinese hamster, rat micronucleus test negative (10).

Other effects

Other adverse effects (human)

A diabetic woman treated with $0.5 \text{ g } 2 \times \text{day}^{-1}$ gave birth to an infant with a severe teratology of Fallot (a form of congenital heart disorder) which died within 1 wk (11).

Adverse effects include nausea, vomiting, heartburn, diarrhoea, increased appetite and weight gain, hypoglycaemia, and occasionally increased secretion of antidiuretic hormone causing water retention, hyponatraemia and central nervous system effects (12).

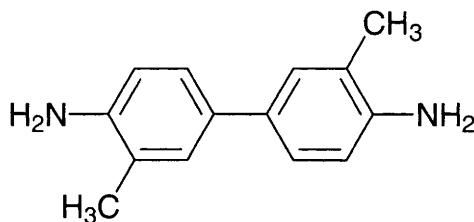
An increased incidence in mortality from cardiovascular complications has been reported in diabetics given tolbutamide compared with other treatments (13-16).

A non-diabetic woman who ingested 25-30 g with suicidal intent developed hypoglycaemic coma, with brain damage and death from pneumonia after 5 months without regaining consciousness (17).

References

1. *Int. J. Crude Drug Res.* 1988, **26**, 81.
2. *Prog. Med. Chem.* 1961, **1**, 187.
3. *Nature* 1962, **193**, 891.
4. *Pharm. Chem. J. (Eng. Trans.)* 1980, **14**, 107.
5. *Farmacol. Ed. Sci.* 1957, **12**, 268.
6. *Prog. Med. Chem.* 1961, **1**, 187.
7. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-PB274483/AS, NIEHS, Research Triangle Park, NC, USA.
8. Miller, A. K. et al *Eur. J. Clin. Pharmacol.* 1990, **38**(5), 523-524.
9. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
10. Renner, H. W. et al *Mutat. Res.* 1980, **77**, 349-355.
11. Coopersmith, H. et al *Can. Med. Assoc. J.* 1962, **87**, 193.
12. Paice, B. J. et al *Adv. Drug React. Acute Poisoning Rev.* 1985, **4**, 23-36.
13. *JAMA, J. Am. Med. Assoc.* 1971, **218**, 1400-1410.
14. *JAMA, J. Am. Med. Assoc.* 1971, **217**, 777-784.
15. *JAMA, J. Am. Med. Assoc.* 1975, **231**, 583-600.
16. *FDA Drug Bull.* 1984, **14**, 16-17.
17. Lazner, J. *Med. J. Austr.* 1970, **i**, 327-328

T172 o-tolidine



C₁₄H₁₆N₂

Mol. Wt. 212.29

CAS Registry No. 119-93-7

Synonyms 3,3'-dimethylbenzidine; 3,3'-dimethyl-[1,1'-biphenyl]-4,4'-diamine; C.I. 37230; C.I. Azoic Diazo Component 113; Fast Dark Blue Base R; 3,3'-tolidine

EINECS No. 204-358-0

RTECS No. DD 1225000

Uses Formerly used as analytical reagent. Manufacture of dyestuffs.

Physical properties

M. Pt. 129-131°C **B. Pt.** 300°C **Specific gravity** 1.0 at 20°C **Partition coefficient** $\log P_{ow}$ 2.34 (1)
Solubility Water: slightly soluble. Organic solvents: acetic acid, chloroform, diethyl ether, ethanol

Occupational exposure

UN No. 1708 **HAZCHEM Code** 3X **Conveyance classification** toxic substance

Supply classification toxic, dangerous for the environment

Risk phrases May cause cancer – Harmful if swallowed – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R45, R22, R51/53)

Safety phrases Avoid exposure – obtain special instruction before use – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet - Restricted to professional users (S53, S45, S61)

Ecotoxicity

Invertebrate toxicity

EC₅₀ (24 hr) *Daphnia magna* 3.2 mg l⁻¹. 21 day reproduction test NOEC 0.16 mg l⁻¹ (nominal value) (2).

Cell multiplication inhibition test *Scenedesmus subspicatus* EC₁₀ 0.75 mg l⁻¹, test period 0-72 hr (3).

Bioaccumulation

Calculated bioconcentration factor 35.

Environmental fate

Degradation studies

99-100% removal from waste-water by activated sludge process at 20 mg l⁻¹ after 6 hr at 25°C (4).

Abiotic removal

t_{1/2} for reaction with photochemically produced hydroxyl radicals in the atmosphere 4 hr (5).

Adsorption and retention

Estimated K_{oc} 447 indicates a tendency to absorb to organic matter (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 405 mg kg⁻¹ (6).

LD_{Lo} intraperitoneal rat, mouse 125 mg kg⁻¹ (7).

Carcinogenicity and chronic effects

No adequate evidence for evaluation of carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2B (8).

Oral mouse (27 month) 0, 5, 9, 18, 35, 70 or 140 mg l⁻¹ of the dihydrochloride in drinking water. Fatal lung alveolar cell neoplasms appeared in ♂ mice receiving 140 mg l⁻¹ at 78 wk. There were no significant treatment-related trends for this neoplasm in ♀ mice, nor in body weight or other lesions in either sex (9).

Subcutaneous rat (2 yr) 60 mg wk⁻¹ (total dose 5.5 g). Five rats developed cancer of the external auditory canal. None of these tumours occurred in untreated animals (10).

Subcutaneous rat (13 month) 20 mg wk⁻¹ for 13 month. 30/50 animals developed a total of 41 tumours, including carcinomas of the Zymbal gland (11).

Gavage ♀ rat (9 month) 500 mg at 3 day intervals. 3/16 developed mammary tumours (12).

Metabolism and toxicokinetics

Readily absorbed through the skin of mammals (13).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535 with and without metabolic activation positive (14).

In vitro L5178Y tk⁺/tk⁻ mouse lymphoma cells, with and without metabolic activation positive (15).
In vitro rat and hamster hepatocytes, DNA repair assay positive (16).
In vitro Chinese hamster ovary cells, sister chromatid exchanges and chromosomal aberrations positive (17).

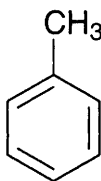
Other comments

Physical properties, use, carcinogenicity and metabolism reviewed (12,13).
 Environmental fate, ecotoxicity and toxicity reported (18-20).

References

1. Hansch, L. et al *Medchem Project Issue No. 26* 1985, Pomona College, Claremont, CA, USA.
2. Kuehn, R. et al *Water Res.* 1989, **23**(4), 501-510.
3. Kuehn, R. et al *Water Res.* 1990, **24**(1), 31-38.
4. Baird, R. et al *J. Water Pollut. Control Fed.* 1977, **49**(7), 1609-1615.
5. Jaber, H. M. et al *Data Acquisition for Environmental Transport and Fate*. 1984, USEPA-600/6-84-011.
6. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, 72, Prague, Czechoslovakia.
7. *Summary Tables of Biological Tests* 1954, **6**, 64.
8. *IARC Monograph* 1987, **Suppl. 7**, 62.
9. Schieferstein, G. J. et al *Food Chem. Toxicol.* 1989, **27**(12), 801-806.
10. Spitz, S. et al *Cancer (Philadelphia)* 1950, **3**, 789.
11. Pliss, G. B. et al *J. Natl. Cancer Inst.* 1970, **45**, 283.
12. *IARC Monograph* 1972, **1**, 87-91.
13. *Chemical Safety Data Sheets* 1991, **4b**, 213-216, The Royal Society of Chemistry, London, UK.
14. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-158.
15. Mitchell, A. D. et al *Environ. Mol. Mutagen.* 1988, **12**(Suppl. 13), 37-101.
16. Corbett, M. D. et al *Chem.-Biol. Interact.* 1987, **63**(3), 249-264.
17. Galloway, S. M. et al *Environ. Mol. Mutagen.* 1987, **10**(Suppl. 12), 1-175.
18. Haltrich, W. G. *Vom Wasser* 1989, **73**, 11-24 (Ger.) (*Chem. Abstr.* 112 124566q).
19. *Gov. Rep. Announce. Index (U. S.)* 1989, **89**(3), Abstr. No. 906602.
20. Walton, B. T. et al *NTIS Report ORNL-6451* 1989, 1-285, Order No. DE89016892, Oak Ridge, TN, USA

T173 toluene



C₇H₈

Mol. Wt. 92.14

CAS Registry No. 108-88-3

Synonyms methylbenzene; CP25; methyl acide; methylbenzol; phenylmethane; toluol

EINECS No. 203-625-9

RTECS No. XS 5250000

Uses In the manufacture of benzoic acid, benzaldehyde, explosives, dyes. Solvent for paints, lacquers, gums and resins. Gasoline additive. In extraction of various principles from plants.

Occurrence In coal tar.

Physical properties

M. Pt. -93°C **B. Pt.** 110.6°C **Flash point** 4.4°C (closed cup) **Specific gravity** 0.866 at 30°C with respect to water at 4°C **Partition coefficient** log P_{ow} 2.73 **Volatility** v.p. 36.7 mmHg at 30°C; v.den. 3.14

Solubility Water: 0.067% w/w at 23.5°C. Organic solvents: acetone, carbon disulfide, chloroform, diethyl ether, ethanol, glacial acetic acid

Occupational exposure

DE-MAK 50 ppm (190 mg m⁻³)

FR-VME 100 ppm (375 mg m⁻³)

JP-OEL 50 ppm (188 mg m⁻³)

SE-LEVL 50 ppm (200 mg m⁻³)

UK-LTEL 50 ppm (191 mg m⁻³)

US-TWA 50 ppm (188 mg m⁻³)

FR-VLE 150 ppm (550 mg m⁻³)

SE-STEL 100 ppm (400 mg m⁻³)

UK-STEL 150 ppm (574 mg m⁻³)

UN No. 1294 **HAZCHEM Code** 3/E **Conveyance classification** flammable liquid

Supply classification highly flammable, harmful

Risk phrases Highly flammable – Harmful by inhalation (R11, R20)

Safety phrases Keep out of reach of children (if sold to general public) – Keep away from sources of ignition – No smoking – Avoid contact with the eyes – Do not empty into drains – Take precautionary measures against static discharges (S2, S16, S25, S29, S33)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) juvenile striped bass, bluegill sunfish 0.0054, 24 mg l⁻¹, respectively (1,2).

LC₅₀ (48 hr) goldfish 58 mg l⁻¹ (3).

LC₅₀ (96 hr) pink salmon, striped bass, fathead minnow, bluegill sunfish 6.41, 7.3, 12.6, 13.0 mg l⁻¹, respectively (4-7).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 19.7 ppm Microtox test (8).

EC₅₀ (48 hr) *Daphnia magna* 19.6 mg l⁻¹ (6).

LC₅₀ (24 hr) *Palaemonetes pugio*, *Artemia salina*, *Nitocra spinipes* 17.2, 33, 24.2-74.2 mg l⁻¹, respectively (9,10).

Bioaccumulation

The log P_{ow} value indicates slight to moderate accumulation (11).

Eels kept in sea water containing 1.6 mg l⁻¹ had mean concentrations in muscle and liver tissue of 12.4 and 1.5 mg kg⁻¹, respectively; t_{1/2} 1.4 days (12).

It is unlikely that toluene accumulates in an ecosystem food chain (11).

Environmental fate

Nitrification inhibition

Limiting concentration for the inhibition of nitrification (agar test) was 350 mg l⁻¹ (13).

Carbonaceous inhibition

440 mg l⁻¹ did not affect sludge digestion, but at 870 mg l⁻¹ gas production in the digester was reduced by 14.5% (5).

Degradation studies

BOD 65% ThOD in conventional wastewater treatment, 5 day test (3).

Easily degraded by activated sludge in sewage plants (11).

Total toluene loss by biodegradation from oligotrophic lakes, eutrophic lakes, clean rivers, turbid rivers and ponds 0.31, 4.81, 0.36, 0.09 and 18.47%, respectively (3,14,15).

38% of toluene in a mixed culture with *Pseudomonas* sp. was degraded after 180 min (16).

Toluene is biodegraded by a variety of soil microorganisms using the compound as the sole source of carbon (17,18).

Incubation with natural flora in groundwater (with other components of high octane gasoline 100 µl l⁻¹) 100% biodegraded after 192 hr at 13°C, initial concentration 2.22 µl l⁻¹ (19).

Abiotic removal

Reacts with atmosphere free radicals, primarily hydroxyl radicals $t_{1/2}$ 12.8 hr (9,20,21).

40-80% of 0.9 and 0.2 mg l⁻¹ applied to the surface of sandy soils volatilised; $t_{1/2}$ 4.9 hr (9,18).

Adsorption and retention

Adsorbed onto clay minerals following Freundlich's adsorption isotherm. Adsorption capacity increased as pH value decreased (22).

K_{oc} 37-250 (23).

Mammalian & avian toxicity**Acute data**

LD₅₀ oral rat 5000 mg kg⁻¹ (24).

LC₅₀ (8 hr) inhalation mouse 5320 ppm (25).

LC_{Lo} (4 hr) inhalation rat 4600 ppm (26).

LD₅₀ dermal rabbit 12,124 mg kg⁻¹ (26).

LD₅₀ intraperitoneal mouse 640 mg kg⁻¹ (27).

Sub-acute and sub-chronic data

Mice exposed to 2750 mg m⁻³ for 20 days had leukocytosis and decreased thrombocyte and red blood cell counts. There was some evidence of hypoplasia in bone marrow (28).

Mice exposed to 45 g m⁻³ in cycles at 10 min inhalation with 20 min recovery periods, 7 cycles day⁻¹, 5 days wk⁻¹ for 8 wk had depressed body-weight gain, ataxia, immobility, drowsiness, and became unconscious at levels >150 g l⁻¹. Blood-urea nitrogen levels were reduced during exposure. Recovery occurred 2 wk after exposure. Substantial toluene residues were found in the brain after 1 hr (29,30).

Increasing numbers of casts were observed in the collecting tubules of kidneys of rats inhaling 750, 2250, 9375 and 18,570 mg m⁻³ for 5 or 15 wk (31).

♂ Sprague-Dawley rats exposed to 3750 mg m⁻³, 8 hr day⁻¹ for 4 wk had increased adrenal weights after 2 wk and increased eosinophil count after 4 wk (32).

Oral ♀ rat 590 mg kg⁻¹ for up to 6 months showed no adverse effects (33).

Carcinogenicity and chronic effects

National Toxicology Program tested rats and mice via inhalation. No evidence of carcinogenicity found in either species (34).

♂, ♀ Fischer-344 rats were exposed to 0, 112, 375 and 1125 mg m⁻³ 6 hr day⁻¹, 5 × wk⁻¹ for 24 months. ♀ rats exposed to 375 or 1125 mg m⁻³ had a slight but significant reduction in haematocrit. At 1125 mg m⁻³ the mean corpuscular haemoglobin concentration was increased. No histopathological changes were observed and there was no increased frequency of neoplasms compared with controls (35).

One skin papilloma and one skin carcinoma were reported in two different mice out of 30 subjected to topical applications of 16-20 µl 2 × wk⁻¹ for 72 wk (36).

11/35 mice treated with toluene after tumour initiation with 7,12-dimethylbenz[*a*]anthracene had 6 permanent and 5 regressing skin papillomas, indicating some weak promoting activity (37).

Teratogenicity and reproductive effects

4/12 ♂ rats exposed to 750 mg m⁻³, 8 hr day⁻¹, 6 day wk⁻¹ for 1 yr had degeneration of germinal cells of testes.

Rats exposed to 375, 750 mg m⁻³ for 1 yr had decreased absolute testicular weight compared with controls (38).

CFY ♀ rats were exposed to 6000 mg m⁻³ for 24 hr day⁻¹ for days 1-8, 9-14 or 9-21 of pregnancy. No teratogenic effects were observed, but dose-related embryotoxic effects were seen, including increased resorption, decreased foetal and placental weights, and retarded bone development (39).

A significant increase in embryo mortality and decreased foetal weight were observed in mice whose dams were given 0.3-1.0 mg kg⁻¹ by gavage on days 6-15 of gestation. At 1.0 mg kg⁻¹ offspring also had an increased incidence of cleft palate which was not related to growth-rate retardation (40).

New Zealand rabbits exposed to 500 or 1000 mg m⁻³ 24 hr day⁻¹ or day 6-20 of pregnancy caused spontaneous abortions at 1000 mg m⁻³, but no teratogenic effects (41).

Inhalation pregnant CD-1 mice exposed to 200, 400, or 2000 ppm toluene for 60 min three times day⁻¹ during gestational days 12-17. No differences were observed in maternal weight-gain or food consumption between

exposed and control animals. Initial litter characteristics (gestation length, number of litters delivered, litter size) were also similar, but pup weights at birth were lower at 2000 ppm exposure. Pups were evaluated on post-natal days 1-20. Pups exposed to 2000 ppm gained less weight and performed more poorly on behavioural tests than controls or those exposed to 200 or 400 ppm toluene, providing evidence of neurobehavioural teratogenicity of prenatal exposure to high levels of toluene late in gestation. This exposure regime of intermittent high-concentration exposure was designed to simulate human exposures that might occur with toluene, and the results are consistent with case reports of adverse consequences of inhalant abuse by pregnant women (42).

Gavage ♀ rats received toluene in corn oil on days 6-19 of gestation. Controls received corn oil alone. Toluene administered prior to the time of the brain growth spurt caused changes to the brain that were, for the most part, reversible. Exposures after that point resulted in reduced forebrain myelination that may be permanent (43).

Metabolism and toxicokinetics

Rapidly absorbed from the respiratory tract with uptake of 40-60% of the amount inhaled in humans, 90% in dogs (44-48).

Absorbed through the skin in humans, 14-23 mg cm⁻² hr⁻¹ (49,50).

On the basis of measurements of toluene excreted in expired air and hippuric acid in urine of rabbits, toluene appears to be completely absorbed from the gastro-intestinal tract (51,52).

High levels of radioactivity were found in adipose tissue, bone marrow, spinal nerves, spinal cord and white matter of the brain in mice exposed to methyl-¹⁴C-toluene by inhalation. All radioactivity disappeared from nervous tissues within 1 hr and most from body fat within 4 hr (53).

Highest concentrations of radioactivity in adult ♂ rats exposed for 1 hr to ¹⁴C-labelled toluene by inhalation (1950 mg m⁻³) were in the adipose tissues and were 2 orders of magnitude higher than in the blood (46,54).

In humans and laboratory mammals, toluene is converted into benzylalcohol by P₄₅₀ enzymes in the liver. This is then metabolised to benzaldehyde, and then to benzoic acid. Liver enzymes activate benzoic acid to form a co-enzyme A derivative which reacts with glycine to form hippuric acid. 70% of absorbed toluene from the lungs is excreted as hippuric acid in urine within 12 hr. Benzoic acid also reacts with glucuronic acid to form benzoyl glucuronide (55,56).

P₄₅₀ enzymes also convert toluene into *o*- and *p*-cresol, which conjugate with sulfate or glucuronic acid and are then excreted in urine (56).

A study of human volunteers found that hippuric acid excretion was proportional to exposure (57).

Recent evidence suggests that Japanese, and possibly other Asian populations, have a defective gene for aldehyde dehydrogenase and therefore have a defective rate of toluene metabolism (58).

Irritancy

Toluene applied to the eyes of rabbits caused slight irritation but no corneal injury (dose and duration unspecified) (59).

Dermal rabbit (72 hr) 500 mg caused moderate irritation and 2 mg instilled into rabbit eye (24 hr) caused severe irritation (60,61).

Sensitisation

Species sensitivity decreases in the order rabbit, guinea pig, mouse, rat (11).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538 with and without metabolic activation negative (62).

Escherichia coli WP2s with and without metabolic activation negative (62).

In vitro Chinese hamster ovary cells with and without metabolic activation sister chromatid exchange negative, chromosomal aberrations negative (62).

In vitro human lymphocyte cells without metabolic activation sister chromatid exchanges negative, chromosomal aberrations negative (63).

In vitro mouse lymphoma L5178Y tk⁺/tk⁻ positive and negative results reported (64,65).

Drosophila melanogaster sex linked recessive lethal mutations negative, aneuploidy test positive (62).

In vivo mouse bone marrow micronucleus test positive and negative results reported (66,67).

In vivo rat bone marrow chromosomal aberrations positive and negative results reported (68,69).

In vivo ♂ SHR mouse dominant lethal effects negative (70).

Other effects

Other adverse effects (human)

Workers exposed to toluene, benzene and xylene had significantly lower serum IgG and IgA levels (71).

Persons with high body fat content may be exposed to a more prolonged effect of toluene on the central nervous system than thin individuals due to the slow disappearance from adipose tissue and blood (11).

Effects of short-term toluene exposure can be summarised as fatigue and drowsiness up to 375 mg m⁻³ for a few hours; mild throat and eye irritation, some impairment of cognitive functions, headache, dizziness and a sensation of intoxication up to 750 mg m⁻³ for 8 hr; lachrymation, skin paraesthesia, gross incoordination and mental confusion up to 1500 mg m⁻³ for 8 hr (11).

May be used for solvent abuse. Sniffers experience an excitatory stage of drunkenness, dizziness, euphoria, delusions, nausea, vomiting and sometimes visual and auditory hallucinations, followed by central nervous system depression causing confusion, disorientation, headache, blurred vision, reduced speech, drowsiness, muscular incoordination, ataxia, depressed reflexes and nystagmus. In severe cases there is loss of consciousness associated with convulsions (72).

A group of women occupationally exposed to toluene exhibited a relatively high incidence of menstrual disorders and their newborn children experienced more frequent foetal asphyxia, were more often underweight and nursed more poorly (73).

A 22-yr-old man exposed heavily to toluene-based paint developed extensive chemical burns on 71% of his body surface, followed by acute renal failure and disseminated intravascular coagulation resulting in death. The burns were similar to second-degree thermal burns (74).

Any other adverse effects

Mice exposed to 2.5-500 ppm for 5 days exhibited increased sensitivity to respiratory infection by *Streptococcus zooepidemicus* (75).

Rats were exposed to 37,500 mg m⁻³ for 20 min or to 75,000 mg m⁻³ for 1 hr. Decreased mobility was seen at the highest dose, but no quivering, twitching or hyper-response to auditory stimuli (76).

Legislation

Included in Schedules 4 and 6 (Release into the Air/Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (77).

Other comments

NIOSH has designated toluene an ototoxin. It can cause hearing loss, ringing in the ears or total deafness and its toxicity can be exacerbated by combined exposure with noise (78).

Detected in ambient air, cigarette smoke, food and water (11).

Detected in rain water at 0.13-0.7 µg l⁻¹ (79).

Reviews on human health effects, experimental toxicology, environmental effects, workplace exposure, physico-chemical properties, ecotoxicology and epidemiology listed (80).

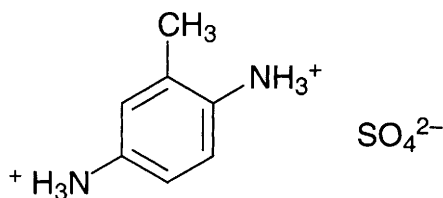
References

1. Palawski, D. et al *Trans. Am. Fish Soc.* 1985, **114**, 748-753.
2. Pickering, Q. H. et al *J. Water Pollut. Control Fed.* 1966, **38**, 1419-1429.
3. Bridie, A. L. et al *Water Res.* 1979, **13**, 623.
4. Korr, S. et al *Bull. Environ. Contam. Toxicol.* 1979, **21**, 521-525.
5. Verschuere, K. *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, Van Nostrand Reinhold, New York, NY, USA.
6. Pearson, J. G. et al *Aquatic Toxicology ASTM 667* 1979, Marking, L. L. et al (Eds.), 284-301.
7. Buccafaso, R. J. *Bull. Environ. Contam. Toxicol.* 1981, **26**, 446.
8. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
9. Little, A. D. (Ed.) *Stored Water Quality Information System* 1980 US Environmental Protection Agency, Washington, DC, USA.
10. Potera, G. T. *Diss. Abstr. B.* 1975, **36**(5), 2010.
11. *IPCS Environmental Health Criteria No. 52 Toluene* 1985, WHO, Geneva, Switzerland.

12. Ogata, M. et al *Water Res.* 1978, **12**(2), 1041-1044.
13. Blok, J. *H₂O* 1981, **14**(11), 242-245.
14. Price, K. S. et al *J. Water Pollut. Control Fed.* 1974, **46**(1), 63-77.
15. Davis, E. M. et al *Water Res.* 1981, **15**, 1125-1127.
16. Chambers, C. W. et al *Water Pollut. Control Fed.* 1974, **46**, (1), 63-77.
17. Kaplan, D. L. et al *Soil Biol. Biochem.* 1979, **11** 335-338.
18. Wilson, J. T. et al *J. Environ. Qual.* 1981, **40**, 501-506.
19. Jamison, V. W. et al *Proc. Third Int. Biodeg. Symp.* 1976, Applied Science Publishers.
20. Brown, S. L. et al *NTIS Report PB263161*, 1975, Natl. Tech. Inf. Ser., Springfield, VA, USA.
21. Perry, R. A. et al *J. Phys. Chem.* 1977, **81**(4), 296-403.
22. El-Dib, M. A. et al *Water Res.* 1978, **12**, 1131-1137.
23. *Hazardous Substances Data Bank* 1993, National Library of Medicine, Washington, DC, USA.
24. *AMA, Arch. Ind. Health* 1959, **19**, 403.
25. *J. Ind. Hyg. Toxicol.* 1943, **25**, 366.
26. *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 470.
27. *Am. N. Y. Acad. Sci.* 1975, **243**, 104.
28. Horiguchi, S. et al *J. Toxicol. Sci.* 1977, **2**(4), 363-372.
29. Bruckner, J. V. et al *Toxicol. Appl. Pharmacol.* 1981, **61**, 27-38.
30. Bruckner, J. V. et al *Toxicol. Appl. Pharmacol.* 1981, **61**, 302-312.
31. Von Oettingern, W. F. et al *The toxicity and potential dangers of toluene with special reference to its maximal permissible concentration* 1942, Bulletin No. 279, US Public Health Service.
32. Takeuchi, Y. et al *Arch. Hig. Rada Toksikol.* 1979, **30**(Suppl.), 467-475.
33. Wolf, M. A. et al *Arch. Ind. Health* 1956, **14**, 387-398.
34. *National Toxicology Program Research and Testing Division Report No. PB90256371*, 1997, NIEHS, Research Triangle Park, NC, USA.
35. Gibson, J. E. et al *Fundam. Appl. Toxicol.* 1983, **3**, 315-319.
36. Lijinski, W. et al *Z. Krebsforsch.* 1972, **77**, 226-230.
37. Frei, J. V. et al *Br. J. Cancer* 1968, **22**, 83-92.
38. Matsumoto, T. et al *Sangyo Igaku* 1971, **13**, 501-506.
39. Hudak, A. et al *Munkavedelem* 1977, **23**(Suppl. 1-3), 25-30.
40. Nawrot, P. S. et al *Teratology* 1979, **19**, 41A.
41. Ungvary, G. U. et al *Proc. 25th Congress Euro. Soc. Toxicol., Budapest* 1984, (No. 134).
42. Jones, H. E. et al *Neurotoxicol. Teratol.* 1997, **19**(4), 305-313.
43. Gospe, S. M., Jr. *Reprod. Toxicol.* 1998, **12**(2), 119-126.
44. Nomkyama, K. et al *Int. Arch. Arbeitsmed.* 1974, **32**(1-2), 75-83.
45. Astrand, I. *Scand. J. Work Environ. Health* 1975, **1**(4), 199-218.
46. Carlsson, A. et al *Scand. J. Work Environ. Health* 1977, **3**(3), 135-143.
47. *Recommended health-based limits in occupational exposure to selected organic solvents* 1981, WHO, Geneva, Switzerland.
48. Carlsson, A. *Scand. J. Work Environ. Health* 1982, **8**(1), 43-55.
49. Dutkiewicz, T. et al *Arch. Gewerbepath. Gewerbehyg.* 1968, **24**, 253-357.
50. Dutkiewicz, T. et al *Br. J. Ind. Med.* 1968, **25**(3), 243.
51. Smith, J. N. *Biochem. J.* 1954, **56**, 317-320.
52. El Masry, A. M. et al *Biochem. J.* 1956, **64**, 50-56.
53. Bergman, K. *Crit. Rev. Toxicol.* 1983, **12**, 59-118.
54. Pyykko, K. et al *Arch. Toxicol.* 1977, **38**, 169-176.
55. *ATSDR Toxicological Profile for Toluene* 1989, Agency for Toxic Substances and Disease Registry, Atlanta, GA, USA.
56. Wang, R. S. et al *Arch. Toxicol.* 1991, **65**, 39-44.
57. Ogata, M. et al *Br. J. Ind. Med.* 1970, **27**(1), 43-50.
58. Greenberg, M. M. *Environ. Res.* 1997, **72**(1), 1-7.
59. *Acute Eye Application – Albino Rabbits* 1962, ESSO Research and Engineering Company, Falls Church, PA, USA.
60. *Food Chem. Toxicol.* 1982, **20**, 563.
61. Marhold, J. V. *Sbornik Vysledku Toxologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
62. McGregor, D. *Mutat. Res.* 1994, **317**, 213-228.
63. Germer-Smidt, P. et al *Mutat. Res.* 1978, **58**, 313-316.
64. Lebowitz, H. et al *Environ. Mutagen.* 1979, **1**, 172-173.
65. McGregor, D. B. et al *Environ. Mol. Mutagen.* 1988, **12**, 85-154.
66. Gad-el-Karim, M. M. et al *Toxicol. Appl. Pharmacol.* 1986, **85**, 464-477.

67. Mohtasamipiers, E. H. et al *Arch. Toxicol.* 1987, **60**, 460-463.
68. Roh, J. et al *Yonsei Med. J.* 1987, **28**, 297-309.
69. Aristov, V. N. et al *Gig. Tr. Prof. Zabol.* 1981, (7), 33-36.
70. Feldt, E. G. et al *Mutat. Res.* 1985, **147**, 294.
71. Lange, A. et al *Int. Arch. Arbeitsmed.* 1973, **31**, 45-50.
72. Streicher, H. Z. et al *Ann. Intern. Med.* 1981, **94**, 758-762.
73. Syrovadko, O. N. *Gig. Tr. Prof. Zabol.* 1977, (12), 15-19.
74. Shibata, K. et al *Am. J. Emerg. Med.* 1994, **12**(3), 353-355.
75. Aranji, W. et al *Toxicol. Lett.* 1985, **25**, 103-110.
76. Furnas, D. W. et al *Am. Med. Assoc. Arch. Ind. Health* 1958, **18**, 9-15.
77. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
78. *Chem. Health Saf.* 1997, **4**(2), 29.
79. Lahmann, E. et al *Proc. 4th Int. Clean Air Congress* 1977, 595-597.
80. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T174 2,5-toluenediamine sulfate



$C_7H_{12}N_2O_4S$

Mol. Wt. 220.25

CAS Registry No. 6369-59-1

Synonyms 2-methyl-1,4-benzenediamine, sulfate; C.I. 76043; C.I. oxidation base 4; Fouramine STD

EINECS No. 228-871-4

RTECS No. XT 0524000

Uses Used in fur dyeing. In hair dye formulations.

Physical properties

Solubility Organic solvents: ethanol

Occupational exposure

Supply classification toxic

Supply classification dangerous for the environment

Risk phrases Harmful by inhalation and in contact with skin – Toxic if swallowed – May cause sensitisation by skin contact – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R20/21, R25, R43, R50/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Avoid contact with the skin – Wear suitable gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S24, S37, S45, S60, S61)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 98 mg kg⁻¹ (1).

LD₅₀ intraperitoneal rat 49 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

Sprague-Dawley rats were administered 0.75-24 mg kg⁻¹ subcutaneously as a single injection or repeated daily for 3-5 days, or a single intraperitoneal injection of 4-32 mg kg⁻¹. No significant increases in methaemoglobin formation were reported, although some Heinz bodies were found 2-3 day after subcutaneous injections (2).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (2,5-toluenediamine and sulfate) (3).

National Toxicology Program tested rats and mice via gavage. Designated non-carcinogen in both species (4).

No increase in lung tumours compared with controls was observed in Swiss-Webster mice receiving 0.05 ml of a hair dye preparation containing 3% dermally 1 × wk⁻¹ or fortnightly for 18 months (5).

Rats treated with 0.5 g of a formulation containing 4% 2,5-diaminotoluene calculated as free base, but used as sulfate, 2 × wk⁻¹ for 2 yr showed no increased incidence of tumours compared with controls (2).

Sprague-Dawley rats receiving 0.5 ml of a formulation containing 4% 2,5-diaminotoluene sulfate dermally 2 × wk⁻¹ for 2 yr showed no differences in body weight gain, food intake, lifespan, mortality, haematological parameters, liver function or pathological changes compared with controls (2).

Teratogenicity and reproductive effects

20 mated ♀ Charles River CD rats received 2 ml kg⁻¹ of a hair dye formulation containing 3% 2,5-diaminotoluene sulfate on days 1, 4, 7, 10, 13, 16, 19 of gestation. 6/169 live foetuses showed skeletal changes on day 20 of gestation (6).

20 ♀ rats were treated with a formulation containing 6% 2,5-diaminotoluene sulfate. No increase in foetal abnormalities was observed compared with controls (6).

No evidence of embryotoxicity or teratogenicity was observed in rats and rabbits receiving 10, 50, 80 and 10, 25, 50 mg kg⁻¹ day⁻¹ orally on days 6-18 of gestation (7).

♀ mice received 1-1.4 ml 100 g⁻¹ by gavage on days 8-12 of gestation. Mice were allowed to deliver, and neonates were examined, counted and weighed on day 1 and day 3. A significantly high number of dead neonates on day 1 was observed (8).

Metabolism and toxicokinetics

Absorbed through the skin of dogs and excreted in the urine (9).

Six adult humans injected subcutaneously with 10 mg excreted ~50% of the dose within 48 hr as the *N,N'*-diacetyl derivative (10).

Genotoxicity

Salmonella typhimurium TA90, TA100, TA1535, TA15357, TA1538 without metabolic activation negative; with metabolic activation TA1535 negative; TA90, TA100, TA1537, TA1538 some positive response with various types of metabolic activation (11).

Other effects

Other adverse effects (human)

Two patients using hair dyes containing 2,5-diaminotoluene or its sulfate developed aplastic anaemia (12,13).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Sulfates: guide level 25 mg l⁻¹ (14).

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (15).

Other comments

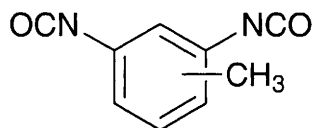
Reviews on human health effects, experimental toxicology, physico-chemical properties listed (16).

References

1. Burnett, C. et al *J. Toxicol. Environ. Health* 1977, 2, 657-662.

2. Kirkel, H. J. et al *Food Cosmet. Toxicol.* 1973, **11**, 641-648.
3. IARC Monograph 1987, **Suppl. 7**, 61.
4. National Toxicology Program Research and Testing Division 1992, Report No. TR-PB287127/AS, NIEHS, Research Triangle Park, NC, USA.
5. Burnett, C. et al *Food Cosmet. Toxicol.* 1975, **13**, 353-357.
6. Burnett, C. et al *J. Toxicol. Environ. Health* 1976, **1**, 1027-1040.
7. Spengler, J. et al *Teratology* 1986, **33**, 31A.
8. Seidenberg, J. M. et al *Teratogen., Carcinogen., Mutagen.* 1986, **6**, 361-374.
9. Kiese, M. et al *Toxicol. Appl. Pharmacol.* 1968, **12**, 495-507.
10. Kiese, M. et al *Toxicol. Appl. Pharmacol.* 1968, **13**, 325-331.
11. Dunkel, V. C. et al *Environ. Mol. Mutagen.* 1985, **7**(Suppl. 5), 1.
12. Hamilton, S. et al *Br. Med. J.* 1976, (ii), 834.
13. Toghill, P. J. et al *Br. Med. J.* 1976, (i), 502-503.
14. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
15. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
16. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T175 toluene diisocyanate



$C_9H_6N_2O_2$

Mol. Wt. 174.16

CAS Registry No. 26471-62-5

Synonyms 1,3-diisocyanatotoluene; 1,3-diisocyanatomethylbenzene; isocyanic acid, methyl-*m*-phenylene ester; methylphenylene isocyanate; TDI; tolylene isocyanate

EINECS No. 247-722-4

RTECS No. NQ 9490000

Uses Plasticiser and component of industrial adhesives and slurries. Precursor of polyurethane.

Occupational exposure

FR-VME 0.01 ppm (0.08 mg m⁻³)

FR-VLE 0.02 ppm (0.16 mg m⁻³)

JP-OEL 0.005 ppm (0.035 mg m⁻³), ceiling limit 0.02 ppm (0.14 mg m⁻³)

SE-LEVL 0.005 ppm

SE-CEIL 0.01 ppm

UK-LTEL MEL 0.02 mg m⁻³ (as NCO)

UK-STEL MEL 0.07 mg m⁻³ (as NCO)

Environmental fate

Degradation studies

Degenerates in moist soil to form polyureas of diisocyanates (1).

Abiotic removal

On contact with water, the compounds may be converted into diaminotoluenes (2).

Mammalian & avian toxicity

Acute data

In vitro causes contraction of rat urinary bladder via release of cyclooxygenase products in a concentration-dependent manner (3).

In vitro compound releases 15-hydroxyeicosatetraenoic acid from human bronchial epithelial cells in a dose-related fashion 8-18 ppb (4).

In vitro compound can enhance response of rat tracheal ring to methacholine at 1 μM (5).

Rats exposed to 0.082-1.087 ppm for 4 hr, showed an increase in the number of polymorphonuclear neutrophils in lung washings, in a dose-related fashion, accompanied by an increase in *N*-acetyl- β -glucosaminidase levels in macrophages (6).

Sub-acute and sub-chronic data

Rats exposed to 0.7-4.3 ppm for 4 hr day⁻¹ for up to 14 days showed local inhibition of acetyl cholinesterase activity in bronchial tissue. Acetyl cholinesterase activity in blood was unaffected (7).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2B (8).

National Toxicology Program tested rats and mice via gavage. ♂ rats showed positive carcinogenic effects including subcutaneous fibromas and fibrosarcomas. ♀ rats showed positive carcinogenic effects including fibroadenomas and mammary tumours. ♀ mice showed positive carcinogenic effects including haemangiomas of the spleen and subcutaneous tissues, hepatic adenomas and haemangiomas of liver, ovaries and peritoneum. ♂ mice showed no evidence of carcinogenicity (9).

Mice inhaling 0.05-0.15 ppm 6 hr day⁻¹, 5 day wk⁻¹ for 104 wk, lost body-weight and some ♀ died. No tumours or respiratory changes were seen. Rats inhaling 0.05-15 ppm 6 hr day⁻¹, 5 day wk⁻¹ for 104 wk showed reduced weight gain, but no tumours or other pathological changes (10).

Genotoxicity

Studies with hepatocytes from livers of rats with induced metabolism, produced negative results in unscheduled DNA synthesis tests (11).

Other comments

Air pollutant.

Causes industrial asthma (5).

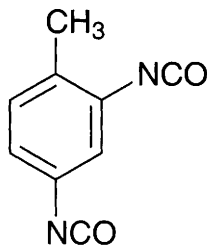
Environmental fate reviewed (1).

Carcinogenicity and toxicology reviewed (10).

References

1. Duff, P. B. *Polyurethane: New Paths Prog., Mark., Technol., Proc. SPI Int./Tech./Mark. Conf.*, 6th 1983, 408-412, New York Soc. of Plastic Industry, San Diego, CA, USA.
2. *IARC Monograph* 1979, **19**, 303-340.
3. Mapp, C. E. *Br. J. Pharmacol.* 1990, **100**(4), 886-888.
4. Mattoli, S. J. *Cell. Physiol.* 1990, **142**(2), 379-385.
5. Born, P. J. A. *Br. J. Ind. Med.* 1989, **46**(1), 56-59.
6. Herbert, A. et al *Toxicol. Lett.* 1991 **56**(1-2), 53-54.
7. Brondeu, M. T. et al *J. Appl. Toxicol.* 1990, **10**(6), 423-427.
8. *IARC Monograph* 1987, **Suppl. 7**, 72.
9. *National Toxicology Programme Research and Testing Division* 1992, Report No. PB7115176, NIEHS, Research Triangle Park, NC, USA.
10. *IARC Monograph* 1986, **39**, 287.
11. Shaddock, J. G. *Mutagenesis* 1990, **5**(4), 387-391

T176 toluene 2,4-diisocyanate



C₉H₆N₂O₂

Mol. Wt. 174.16

CAS Registry No. 584-84-9

Synonyms 2,4-diisocyanato-1-methylbenzene; 4-methyl-*m*-phenylene diisocyanate; 2,4-toluene diisocyanate; 2,4-TDI; tolylene 2,4-diisocyanate; Nacconate 100

EINECS No. 209-544-5

RTECS No. CZ 6300000

Uses Manufacture of polyurethane foams and coatings, urethane elastomers, paints and varnishes. Cross-linking agent.

Physical properties

M. Pt. 22°C **B. Pt.** 251°C **Flash point** 132°C (open cup) **Specific gravity** 1.2244 at 25°C with respect to water at 4°C **Volatility** v.p. 0.01 mmHg at 20°C; v.den. 6.0

Solubility Organic solvents: acetone, benzene, carbon tetrachloride, chlorobenzene, diglycol monomethyl ether, kerosene, olive oil

Occupational exposure

DE-MAK 0.01 ppm (0.072 mg m⁻³)

FR-VME 0.01 ppm (0.08 mg m⁻³)

FR-VLE 0.02 ppm (0.16 mg m⁻³)

JP-OEL 0.005 ppm (0.035 mg m⁻³), ceiling limit 0.02 ppm (0.14 mg m⁻³)

SE-LEVL 0.005 ppm (0.04 mg m⁻³)

SE-CEIL 0.01 ppm (0.07 mg m⁻³)

UK-LTEL MEL 0.02 mg m⁻³ (as NCO)

UK-STEEL MEL 0.07 mg m⁻³ (as NCO)

US-TWA 0.005 ppm (0.036 mg m⁻³)

US-STEEL 0.02 ppm (0.14 mg m⁻³)

UN No. 2078 **HAZCHEM Code** 2XE **Conveyance classification** toxic substance

Supply classification toxic

Risk phrases Toxic by inhalation – Irritating to eyes, respiratory system and skin – May cause sensitisation by inhalation (R23, R36/37/38, R42)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Do not breathe vapour – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – After contact with skin, wash immediately with plenty of water – In case of insufficient ventilation, wear suitable respiratory equipment – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S23, S26, S28, S38, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) fathead minnow 194 mg l⁻¹ (1).

Invertebrate toxicity

Grass shrimp mortality <65% in 96 hr, exposure concentration <508 mg l⁻¹ (1).

Environmental fate

Abiotic removal

The immediate hydrolysis product is 2,4-diaminotoluene (2).

In model river and marine systems hydrolysis occurred within a day (1).

Removal from the atmosphere is due to reaction with photochemically produced hydroxyl radicals ($t_{1/2}$ 3.3 hr), as well as through dry deposition (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird, starling 100, >100 mg kg⁻¹, respectively (2).

LD₅₀ oral rat 5800 mg kg⁻¹ (4).

LC₅₀ (4, 4, 6, 3 hr, respectively) mouse, guinea pig, rat, rabbit 10, 13, 600, 1500 ppm respectively (5-7).

LD₅₀ intravenous mouse 56 mg kg⁻¹ (8).

Sub-acute and sub-chronic data

LC₅₀ inhalation mouse, rat, rabbit, guinea pig (14 day, 4 hr day⁻¹) 10-14 ppm (9).

Carcinogenicity and chronic effects

Toluene diisocyanates: no adequate evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2B (10).

Inadequate evidence for carcinogenicity of toluene 2,4-diisocyanate to humans and animals (11).

A commercial mixture of 2,4- and 2,6-toluene diisocyanate administered by gavage caused multiple tumours in ♂, ♀ rats and ♀ mice. The carcinogenicity was thought to be due to metabolism of the 2,4-TDI to products identical to those from metabolism of 2,4-diaminotoluene, a known carcinogen (12).

Oral ♂, ♀ mice (101 wk) 100 or 200 mg kg⁻¹ diet. Mean body weights of high-dose ♂ animals were reduced compared with controls. No significant difference in survival rates was noted between treated animals and controls. All treated ♀ had an increase in hepatocellular carcinomas; low-dose ♀ also had an increased incidence of lymphomas. No significant increase in tumour incidence was found in ♂ (1).

Oral ♂, ♀ rats (103 wk) 79 mg kg⁻¹ (time-weighted average, low dose ♀ ♂); 171 mg kg⁻¹ (high-dose ♀); and 176 mg kg⁻¹ (high-dose ♂). A dose-related increase in the combined incidence of hepatocellular carcinomas and neoplastic nodules occurred in both sexes, but this was not considered significant except for high-dose ♂. The incidence of subcutaneous tissue fibromas was increased in ♂ and mammary gland carcinomas and adenomas in ♀ (1).

Irritancy

A 10% solution painted into the nasal vestibuli of guinea pigs once a day for 5-10 days induced nasal allergy (13).

To the human eye, 0.35 mg m⁻³ caused irritation and was lachrymatory (14).

Dermal rabbit (24 hr) 500 mg caused moderate irritation and 100 mg instilled into rabbit eye (72 hr) caused severe irritation (15).

Sensitisation

Sensitisation has been reported in humans after a single exposure. It can also develop days, months or years after exposure, and after high level or chronic low level exposure (16).

Respiratory hypersensitivity occurred in guinea pigs after dermal application (17).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1538 with metabolic activation negative (18).

In vitro Chinese hamster ovary cells with metabolic activation chromosomal aberrations and sister chromatid exchanges negative, without metabolic activation sister chromatid exchanges equivocal (19).

In vitro mouse lymphoma L5178Y tk⁺/tk⁻ cell forward mutation assay positive (20).

Other effects

Other adverse effects (human)

Occupational exposure during polyurethane foam manufacture causes general toxicity, allergic and fibrogenic effects in workers (21).

2,4-Diisocyanatotoluene is a strong respiratory irritant and sensitiser and causes asthma attacks, loss of lung function, and two chronic restrictive lung diseases, hypersensitivity pneumonitis and chronic bronchitis (22).

Any other adverse effects

Single or repeated exposures to 0.05-14 mg m⁻³ for <3 hr caused reduced respiratory rates in mice (1).

Bronchopneumonia has been reported in rats following gavage administration. Symptoms include abdominal distress and sickness (17).

Sensitisation, reduced respiratory rate, pneumonitis, tracheitis, bronchitis, necrotic rhinitis and fibrosis in the bronchiole walls and effects on the liver, kidneys, and gastro-intestinal tract have been reported in animal studies (17).

Legislation

Permitted in USA as component of adhesives and polyurethane resins that come into contact with food (23).

Designated by the US EPA as a hazardous waste (24).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Cyanides: maximum admissible concentration 50 µg l⁻¹ (25).

Other comments

Occurs in stock exhaust from polyurethane foam production plant and in waste waters.

Most commercial formulations are as the 80:20 mixture of the 2,4- and 2,6-isomers. Physical properties, uses, occupational exposure, analysis, carcinogenicity, mammalian toxicity and mutagenicity of diisocyanatotoluenes and their hydrolysis products reviewed (2,14,26,27).

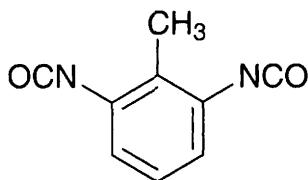
The effects on the lung (28,29) and exposure effects in the polyurethane industry reviewed (30).

References

1. IARC Monograph 1986, **39**, 287-323.
2. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
3. Duff, P. B. *Polythene – New Paths to Progress Marketing Technology* 1983, 408-412.
4. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1989, **1**, 505-511, Lewis Publishers, Chelsea, MI, USA.
5. Kennedy, G. L. et al *Toxicol. Lett.* 1991, **56**(3), 317-326.
6. AMA, *Arch. Ind. Health* 1957, **15**, 324.
7. *Am. Ind. Hyg. Assoc. J.* 1962, **23**, 447.
8. Report No. 07807, US Army Research and Development Command, Chemical Systems Laboratories, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD, USA.
9. Henschler, D. *Toxikol. Arbeitsmed. Begründung. MAK-Werte* Verlag Chemie.
10. IARC Monograph 1987, **Suppl. 7**, 72.
11. IARC Monograph 1979, **19**, 303-340.
12. Dieter, M. B. et al *Toxicol. Environ. Health* 1990, **6**(6), 599-621.
13. Tanaka, K. et al *Int. Arch. Allergy Appl. Immunol.* 1988, **85**(4), 392-397.
14. ICPS Environmental Health Criteria No. 75 *Toluene Diisocyanates* 1987, WHO, Geneva, Switzerland.
15. *Eur. J. Toxicol. Environ. Hyg.* 1976, **9**, 41.
16. Lenga, R. E. *The Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3376, Sigma-Aldrich, Milwaukee, WI, USA.
17. *Chemical Safety Data Sheets* 1991, **4b**, 221-224, The Royal Society of Chemistry, London, UK.
18. Anderson, M. et al *Scand. J. Work Environ. Health* 1980, **6**, 221-226.
19. Gulati, D. K. et al *Environ. Mol. Mutagen.* 1989, **13**(2), 133-193.
20. McGregor, D. B. et al *Environ. Mol. Mutagen.* 1991, **17**(3), 196-219.
21. Platinina, R. A. et al *Gig. Tr. Prof. Zabol.* 1986, (12), 16-20 (Russ.) (*Chem. Abstr.* **106**, 72197z).
22. Baur, X. *Allergologie* 1986, **9**(11), 487-496.

23. *US Code Fed. Regul. Title 21 Parts 175.105, 177.1680, 1984, 137, 256, US Food and Drug Administration, Food and Drugs.*
24. *US Code Fed. Regul. Title 40 Part 261.33, 1984, 364, USEPA, Protection of Environment.*
25. *EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.*
26. *ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.*
27. *IARC Monograph 1978, 16, 83-95.*
28. Karol, M. H. *CRC, Crit. Rev. Toxicol.* 1986, **16**(4), 349-379.
29. Kay, S. *Food Chem. Toxicol.* 1985, **23**(3), 411-413.
30. Burrows, G. E. *Cell. Polym.* 1983, **2**(3), 205-212

T177 toluene 2,6-diisocyanate



$C_9H_6N_2O_2$

Mol. Wt. 174.16

CAS Registry No. 91-08-7

Synonyms 2,6-diisocyanatotoluene; isocyanic acid, 2-methyl-*m*-phenylene ester; 2,6-TDI; 2,6-toluene diisocyanate; tolylene 2,6-diisocyanate; *m*-tolylene 2,6-diisocyanate

EINECS No. 202-039-0

RTECS No. CZ 6310000

Physical properties

M. Pt. 7.2°C (freezing point) B. Pt. 129-133°C at 118 mmHg Specific gravity 1.22

Occupational exposure

DE-MAK 0.01 ppm (0.072 mg m⁻³)

JP-OEL 0.005 ppm (0.035 mg m⁻³), ceiling limit 0.02 ppm (0.14 mg m⁻³)

SE-LEVL 0.005 ppm

SE-CEIL 0.01 ppm

UK-LTEL MEL 0.02 mg m⁻³ (as NCO)

UK-STEL MEL 0.07 mg m⁻³ (as NCO)

UN No. 2078 HAZCHEM Code 2XE Conveyance classification toxic substance

Supply classification toxic

Risk phrases Toxic by inhalation – Irritating to eyes, respiratory system and skin – May cause sensitisation by inhalation (R23, R36/37/38, R42)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Do not breathe vapour – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – After contact with skin, wash immediately with plenty of water – In case of insufficient ventilation, wear suitable respiratory equipment – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S23, S26, S28, S38, S45)

Ecotoxicity

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 41.8 ppm Microtox test (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral blackbird, starling 100 mg kg⁻¹ (2).

LC₅₀ (4 hr) inhalation mouse 91 mg m⁻³ (3).

Teratogenicity and reproductive effects

Intraperitoneal mice 30-100 mg kg⁻¹ showed reduced synthesis of DNA in testes. This may be an indirect effect resulting from lowered body temperature (4).

Irritancy

Powerful irritant to mucous membranes of eye and respiratory tract (5,6,7).

Inhalation human 50 ppb caused irritation to nose, eyes and respiratory system (duration unspecified) (5).

Inhalation mouse (3 hr) 0.007-2 ppb caused sensory irritation of respiratory tract and reduced rate of respiration.

Slow recovery observed (6).

Genotoxicity

Salmonella typhimurium TA98, TA100 with metabolic activation positive (8).

In vivo rat hepatocytes DNA repair test negative after 2 or 12 hr (9).

Other effects

Other adverse effects (human)

One human case of cancer of the respiratory tract has been linked to diisocyanate inhalation (10).

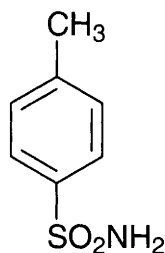
Other comments

Toxicology and human health effects reviewed (11,12).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
2. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
3. Weyel, D. A. et al *Toxicol. Appl. Pharmacol.* 1982, **64**, 423.
4. Greene, E. J. *Mutat. Res.* 1981, **91**, 75-79.
5. *Arch. Toxikol.* 1962, **19**, 364.
6. Sangha, G. K. et al *Toxicol. Appl. Pharmacol.* 1979, **50**, 533-547.
7. Natl. Inst. Occup. Health 1973, H5M73-1102, Dept. Health, Education and Welfare, Washington, DC, USA.
8. Florin, I. et al *Toxicology* 1980, **18**, 219-232.
9. Mirsalis, J. C. et al *Environ. Mol. Mutagen.* 1982, **4**, 553-562.
10. *IARC Monograph* 1979, **19**, 303-340.
11. *IARC Monograph* 1987, **Suppl. 7**, 72.
12. *IARC Monograph* 1986, **39**, 287

T178 *p*-toluenesulfonamide



$C_7H_9NO_2S$

Mol. Wt. 171.22

CAS Registry No. 70-55-3

Synonyms toluene-4-sulfonamide; 4-toluenesulfonamide; 4-MBSA

EINECS No. 200-741-1

RTECS No. XT 5075000

Uses Intermediate in the manufacture of pesticides and drugs. Additive to outdoor paints. Nickel plating brightening agent. Plasticiser (polyamide hot melt adhesives).

Physical properties

M. Pt. 138-139°C **B. Pt.** 221°C at 10 mmHg **Flash point** 202°C (closed cup)

Partition coefficient $\log P_{ow}$ 0.84 at 25°C **Volatility** v.p. 0.75 mmHg at 170°C

Solubility Water: 3.2 g l⁻¹ at 25°C

Ecotoxicity

Fish toxicity

Non-toxic to fish (1).

Invertebrate toxicity

Non-toxic to daphnids, but slightly toxic to algae (1).

Bioaccumulation

Confirmed to be non-accumulative or low accumulative (2).

Environmental fate

Degradation studies

Not readily biodegradable (1).

Slowly biotransformed in anaerobic aquifer slurries under sulfate-reducing and methanogenic conditions (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwinged blackbird and starling 75 mg kg⁻¹ (4).

LD₅₀ intraperitoneal mouse 250 mg kg⁻¹ (5).

Sub-acute and sub-chronic data

Lowest-observed-adverse-effect level in rats for repeated dose toxicity 120 mg kg⁻¹ day⁻¹ (1).

Teratogenicity and reproductive effects

No-observed-adverse-effect level for reproductive toxicity in rats 300 mg kg⁻¹ day⁻¹ (1).

Metabolism and toxicokinetics

Oral rats administered 29 mg kg⁻¹ [¹⁴C]toluene-4-sulfonamide rapidly eliminated 66-89% of the dose in the urine and 2-8% in the faeces. The major metabolite in urine was 4-sulfamoylbenzoic acid (93%), with small amounts of unchanged toluene-4-sulfonamide (1.5-2.3%), 4-sulfamoylbenzyl alcohol (2.0-3.9%), 4-sulfamoylbenzaldehyde (0-1.5%), and at a higher dose (200 mg kg⁻¹) *N*-acetyltoluene-4-sulfonamide (2.1-2.3%) (6).

Genotoxicity

Weakly mutagenic in a modified *Salmonella*/microsome test and in *Drosophila melanogaster* (7).

Other comments

In 3-day feeding tests on 2%-treated white wheat seeds, 70% of house mice refused to eat more than 50% of treated feed (8).

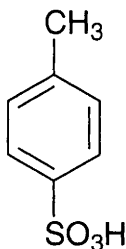
Estimated dose of low concern for man calculated as 0.024 mg kg⁻¹ day⁻¹ and 0.6 mg kg⁻¹ day⁻¹ for repeated dose toxicity and reproductive toxicity, respectively (1).

A high production volume chemical, ~1700 tonnes and 1000 tonnes for 1985 and 1991, respectively, in Japan (1).

References

1. Organisation for Economic Cooperation and Development, *Screening Information Data Set of High Production Chemicals* OECD Chemicals Programme, OECD Paris Centre, 2 rue Andre Pascal, 75775 Paris Cedex, France.
2. *Chemicals Inspection and Testing Institute* 1987, Japan.
3. Kuhn, E. P. et al *Hazard. Waste Hazard. Mater.* 1989, 6(2), 121-123.
4. Schafer, E. W., Jr. *Toxicol. Appl. Pharmacol.* 1972, 21, 315.
5. *Report No. AD691-490* National Technical Information Service, Springfield, VA 22161, USA.
6. Ball, L. M. et al *Xenobiotica* 1978, 8(3), 183-190.
7. Eckhardt, K. et al *Toxicol. Lett.* 1980, 7(1), 51-60.
8. Schafer, E. W., Jr. et al *Arch. Environ. Contam. Toxicol.* 1985, 14(1), 111-129

T179 *p*-toluenesulfonic acid



C₇H₈O₃S

Mol. Wt. 172.20

CAS Registry No. 104-15-4

Synonyms 4-methylbenzenesulfonic acid; tosoic acid; *p*-methylphenylsulfonic acid; *p*-tolylsulfonic acid

EINECS No. 203-180-0

RTECS No. XT 6300000

Uses In dye chemistry. In manufacture of oral antidiabetic drugs.

Physical properties

M. Pt. 106°C (anhydrous); 38°C (metastable form) **B. Pt.** 140°C at 20 mmHg **Flash point** 184°C

Solubility Water: 670 g l⁻¹. Organic solvents: diethyl ether, ethanol

Occupational exposure

UN No. I 2583, II 2584, III 2585, IV 2586 **HAZCHEM Code** alkyl, aryl or toluene sulfonic acids, liquid, with more than 5% free sulfuric acid (I) 2X **HAZCHEM Code** alkyl, aryl or toluene sulfonic acids, solid, with not more than 5% free sulfuric acid (II) 2X **HAZCHEM Code** alkyl, aryl or toluene sulfonic acid, liquid, with not

more than 5% free sulfuric acid, gelling (III) 2X **HAZCHEM Code** alkyl, aryl or toluene sulfonic acid, liquid, with not more than 5% free sulfuric acid, non-gelling (IV) 2R

Supply classification irritant

Risk phrases Irritating to eyes, respiratory system and skin (R36/37/38)

Safety phrases Keep out of reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Wear suitable gloves (S2, S26, S37)

Ecotoxicity

Invertebrate toxicity

A 50% reduction of cell numbers *vs.* controls was observed when *Chlorella vulgaris* was exposed to 245 ppm for 1 day at 20°C (1).

Environmental fate

Degradation studies

Confirmed to be biodegradable (2).

Decomposition by a soil microflora in 24 days (3).

Activated sludge at 20°C with compound as sole carbon source COD 98.7%; 8.4 mg COD g dry inoculum⁻¹ hr⁻¹ (4).

Abiotic removal

Adsorption on Amberlite XAD-2 23% retention efficiency; influent 9 ppm, effluent 6.9 ppm (5).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 400 mg kg⁻¹ (6).

Metabolism and toxicokinetics

In rats is well absorbed by the gastro-intestinal tract following oral administration and is excreted in urine in a day (7).

Irritancy

Irritating to skin, eyes and respiratory system (species unspecified) (7).

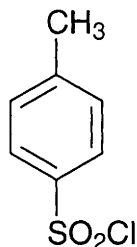
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties, environmental effects, ecotoxicology and exposure levels listed (8).

References

1. Kauss, P. B. et al *Environ. Pollut.* 1975, (9).
2. *The list of the existing chemical substances tested on biodegradability by microorganisms or bioaccumulation in fish body* 1987, Chemicals Inspection and Testing Institute, Japan.
3. Alexander, M. et al *J. Agric. Food Chem.* 1966, **14**, 410.
4. Pitter, P. *Water Res.* 1976, **10**, 231-235.
5. Simpson, R. M. *Progress in hazardous chemicals handling and disposal* 1972, Noyes Data Corp.
6. Patty, F. A. (Ed.) *Industrial Hygiene and Toxicology* 2nd ed., Interscience Publishers, New York, NY, USA.
7. *Chemical Safety Data Sheets* 1990, 3, 260-263, The Royal Society of Chemistry, London, UK.
8. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T180 *p*-toluenesulfonyl chloride



$C_7H_7ClO_2S$

Mol. Wt. 190.65

CAS Registry No. 98-59-9

Synonyms tosyl chloride; toluene-4-sulfonyl chloride; *p*-tolylsulfonyl chloride; *p*-methylphenylsulfonyl chloride; 4-methylbenzenesulfonyl chloride

EINECS No. 202-684-8

Physical properties

M. Pt. 69-71°C **B. Pt.** 146°C at 15 mmHg **Specific gravity** 1.33 **Volatility** v.p. 1 mmHg at 88°C
Solubility Organic solvents: benzene, diethyl ether, ethanol

Occupational exposure

UK-STEL 5 mg m⁻³

Ecotoxicity

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 2.40 ppm Microtox test (1).

Environmental fate

Degradation studies

Confirmed to be biodegradable (2).

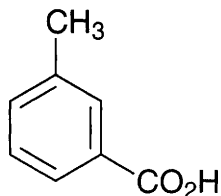
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level 1 µg l⁻¹ (3).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
2. *The list of the existing chemical substances tested on biodegradability by microorganism or bioaccumulation in fish body* 1987, Chemicals Inspection and Testing Institute, Japan.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T181 *m*-toluic acid



$C_8H_8O_2$

Mol. Wt. 136.15

CAS Registry No. 99-04-7

Synonyms 3-methylbenzoic acid; *m*-toluylic acid; *m*-methylbenzoic acid

EINECS No. 202-723-9

RTECS No. XU 1200000

Physical properties

M. Pt. 108-110°C B. Pt. 263°C Specific gravity 1.054 Partition coefficient $\log P_{ow}$ 2.37

Solubility Water: soluble in 1170 parts water at 15°C. Organic solvents: diethyl ether, ethanol

Environmental fate

Degradation studies

Decomposition by a soil microflora in 2 days (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat >3.2 g kg⁻¹ (2).

LD₅₀ oral mouse 1630 mg kg⁻¹ (3).

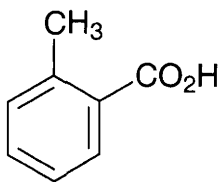
Other comments

Reviews on human health effects, experimental toxicology listed (4,5).

References

1. Alexander, M. et al *J. Agric. Food Chem.* 1966, **14**, 410.
2. Patty, F. A. (Ed.) *Industrial Hygiene and Toxicology* 2nd rev. ed., Interscience Publishers, New York, NY, USA.
3. *Gig. Tr. Prof. Zabol.* 1974, **18**(7), 57.
4. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
5. *BIBRA Toxicity Profiles* 1991, British Industrial Biological Research Association, Carshalton, UK

T182 o-toluic acid



$C_8H_8O_2$

Mol. Wt. 136.15

CAS Registry No. 118-90-1

Synonyms 2-methylbenzoic acid; orthotoluic acid; o-toluylic acid

EINECS No. 204-284-9

RTECS No. XU 1400000

Physical properties

M. Pt. 103-105°C B. Pt. 258-259°C Specific gravity 1.062 Partition coefficient $\log P_{ow}$ 2.46

Solubility Water: soluble in 35 parts boiling water. Organic solvents: chloroform, ethanol

Environmental fate

Degradation studies

Confirmed to be biodegradable (1).

Decomposition by a soil microflora in 16 days (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, rabbit 0.4, 3.32 g kg⁻¹, respectively (3).

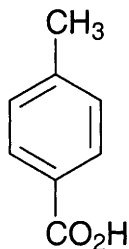
Other comments

Reviews on human health effects, experimental toxicology listed (4,5).

References

1. *The list of the existing chemical substances tested on biodegradability by microorganisms or bioaccumulation in fish body 1987*, Chemicals Inspection and Testing Institute, Japan.
2. Alexander, M. et al *J. Agric. Food Chem.* 1966, **14**, 410.
3. Patty, F. A. (Ed.) *Industrial Hygiene and Toxicology* 2nd rev. ed., Interscience Publishers, New York, NY, USA.
4. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
5. *BIBRA Toxicity Profile* 1991, British Industrial Biological Research Association, Carshalton, UK

T183 *p*-toluic acid



C₈H₈O₂

Mol. Wt. 136.15

CAS Registry No. 99-94-5

Synonyms 4-methylbenzoic acid; crithminic acid; 4-toluic acid

EINECS No. 202-803-3

RTECS No. XU 1575000

Physical properties

M. Pt. 180-182°C B. Pt. 274-275°C Partition coefficient log P_{ow} 2.34

Solubility Water: 12.6 g l⁻¹ at 100°C. Organic solvents: diethyl ether, ethanol, methanol

Environmental fate

Degradation studies

Decomposition by a soil microflora in 8 days (1).

Adsorption and retention

K_{oc} in Podzol acidic forest soil 142; K_{oc} in Alfisol an agricultural soil 14; K_{oc} in a sublimic soil 20 (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 400 mg kg⁻¹ (3).

LD₅₀ oral mouse 2340 mg kg⁻¹ (4).

LD₅₀ intraperitoneal rat, mouse 874, 916 mg kg⁻¹, respectively (4).

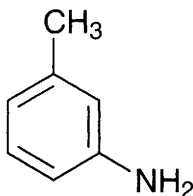
Other comments

Reviews on human health effects, experimental toxicology listed (5,6).

References

1. Alexander, M. et al *J. Agric Food Chem.* 1966, **14**, 410.
2. Von Oepen, B. et al *Chemosphere* 1991, **22**(3-4), 285-304.
3. Patty, F. A. (Ed.) *Industrial Hygiene and Toxicology* 2nd rev. ed., Interscience Publishers, New York, NY, USA.
4. *Kiso to Rinsho* 1978, **12**, 1893.
5. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
6. *BIBRA Toxicity Profile* 1991, British Industrial Biological Research Association, Carshalton, UK

T184 *m*-toluidine



C₇H₉N

Mol. Wt. 107.16

CAS Registry No. 108-44-1

Synonyms 3-methylbenzenamine; 3-aminotoluene; 3-methylaniline; 3-aminophenylmethane; *m*-tolylamine

EINECS No. 203-583-1

RTECS No. XU 2800000

Physical properties

M. Pt. -50°C **B. Pt.** 203-204°C **Flash point** 85°C **Specific gravity** 0.990 at 25°C with respect to water at 25°C

Partition coefficient log P_{ow} 1.40 **Volatility** v.den. 3.72

Solubility Water: slightly soluble in water. Organic solvents: diethyl ether, dilute acids, ethanol

Occupational exposure

US-TWA 2 ppm (8.8 mg m⁻³)

UN No. 1708 **HAZCHEM Code** 3X **Conveyance classification** toxic substance

Supply classification toxic, dangerous for the environment

Risk phrases Toxic by inhalation, in contact with skin and if swallowed – Danger of cumulative effects – Very toxic to aquatic organisms (R23/24/25, R33, R50)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – After contact with skin, wash immediately with plenty of water – Wear suitable protective clothing and gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S28, S36/37, S45, S61)

Ecotoxicity

Fish toxicity

Exposure to 5 ppm was non-toxic to bluegill sunfish, yellow perch and goldfish. Test conditions: temperature 30°C; dissolved oxygen 7.5 ppm; total hardness (soap method) 300 ppm; alkalinity 310 ppm (methyl orange); free carbon dioxide 5 ppm (1).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 11.7 ppm Microtox test (2).

EC₅₀ (16 day) *Daphnia magna* 0.043 mg l⁻¹ (3).

LC₅₀ (48 hr) *Daphnia magna* 0.73 mg l⁻¹ (3).

Environmental fate

Degradation studies

Decomposition by a soil microflora in 8 days (4).

Activated sludge at 20°C with the compound as sole carbon source COD 97.7%; 30 mg COD g dry inoculum⁻¹ hr⁻¹ (5).

Degradation by *Aerobacter* 500 mg l⁻¹ at 30°C; parent strain 100% ring disruption in 62 hr, mutant strain 100% ring disruption in 10 hr (6).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird, quail 242, 562 mg kg⁻¹, respectively (7).

LD₅₀ oral starling >1000 mg kg⁻¹ (7).

LD₅₀ oral rat, mouse 450, 740 mg kg⁻¹, respectively (8,9).

LD₅₀ intraperitoneal mouse 116 mg kg⁻¹ (10).

Irritancy

Dermal rabbit (24 hr) 500 mg caused irritation and 20 mg instilled in rabbit eye (24 hr) caused moderate irritation (11).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538, D3052, C3076, G46 with and without metabolic activation negative (12).

Escherichia coli WP2, WP2uvrA⁻ with and without metabolic activation negative (12).

In vitro primary rat hepatocytes unscheduled DNA synthesis negative (12).

Other comments

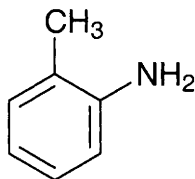
Reviews on human health effects, experimental toxicology, physico-chemical properties, workplace experience, environmental effects, ecotoxicology, exposure levels listed (13).

Autoignition temperature 508°C.

References

1. *The Toxicology of 3400 Chemicals to Fish* 1987, EPA560/6-87-002 PB 87-200-275, Washington, DC, USA.
2. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
3. Hermens, J. et al *Aquat. Toxicol.* 1984, **5**(2), 145-154.
4. Alexander, M. et al *J. Agric. Food Chem.* 1966, **14**, 410.
5. Pitter, P. *Water Res.* 1976, **10**, 231-235.
6. Worne, H. E. *Tijdschrift van het BECEWA*, Liege, Belgium.
7. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
8. *J. Pharmacol. Exp. Ther.* 1947, **90**, 260.
9. *Gig. Tr. Prof. Zabol.* 1981, **25**(8), 50.
10. *Arch. Ital. Sci. Farmacol.* 1951, **1**, 284.
11. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
12. Thompson, C. Z. et al *Environ. Mutagen.* 1983, **5**, 803-811.
13. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T185 o-toluidine



C₇H₉N

Mol. Wt. 107.16

CAS Registry No. 95-53-4

Synonyms 2-methylbenzenamine; 2-aminotoluene; 2-methylaniline; o-tolylamine; 2-toluidine; C.I. 37077; C.I. Azoic Brown 29 (component)

EINECS No. 202-429-0

RTECS No. XU 2975000

Uses Dye intermediate. Used in production of rubber chemicals, pharmaceuticals and pesticides.

Physical properties

M. Pt. -14.7°C (β-form) **B. Pt.** 200-202°C **Flash point** 85°C (closed cup) **Specific gravity** 1.008 at 30°C with respect to water at 20°C **Partition coefficient** log P_{ow} 1.32 **Volatility** v.p. 0.1 mmHg at 20°C; v.den. 3.72 **Solubility** Water: 16.6 mg l⁻¹ at 25°C. Organic solvents: diethyl ether, dilute acids, ethanol

Occupational exposure

FR-VME 2 ppm (9 mg m⁻³)

JP-OEL 1 ppm (4.4 mg m⁻³)

UK-LTEL MEL 0.2 ppm (0.89 mg m⁻³)

US-TWA 2 ppm (8.8 mg m⁻³)

UN No. 1708 **HAZCHEM Code** 3X **Conveyance classification** toxic substance

Supply classification toxic

Supply classification dangerous for the environment

Risk phrases May cause cancer – Toxic by inhalation and if swallowed – Irritating to the eyes – Very toxic to aquatic organisms (R45, R23/25, R36, R50)

Safety phrases Avoid exposure – obtain special instruction before use – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet - Restricted to professional users (S53, S45, S61)

Ecotoxicity

Fish toxicity

LC₅₀ (duration unspecified) fathead minnow, rainbow trout, bluegill sunfish 25.3, 21.97, 22.38 mg l⁻¹, respectively (1).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 13.2 ppm Microtox test (2).

Cell multiplication inhibition test *Pseudomonas putida* 16 mg l⁻¹, *Scenedesmus quadricauda* 6.3 mg l⁻¹, *Entosiphon sulcatum* 76 mg l⁻¹ (3).

LC₅₀ (duration unspecified) *Daphnia magna* 22 mg l⁻¹ (1).

Environmental fate

Degradation studies

ThOD 2.54 g O₂ g⁻¹; BOD₅ 0.242 g O₂ g⁻¹ (4).

Decomposition by a soil microflora >64 days (5).

Adapted activated sludge at 20°C with compound as sole carbon source COD 97.7%; 15.1 mg COD g dry inoculum⁻¹ hr⁻¹ (6).

Degradation by *Aerobacter* 500 mg l⁻¹ at 30°C; parent strain 100% ring disruption in 64 hr, mutant 100% ring disruption in 6 hr (7).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird, starling 100, 422 mg kg⁻¹, respectively (8).

LD₅₀ oral quail >1000 mg kg⁻¹ (8).

LD₅₀ oral mouse, rat, rabbit 520, 670, 840 mg kg⁻¹, respectively (9).

LD_{Lo} oral cat 150 mg kg⁻¹ (10).

LD₅₀ dermal rabbit 3250 mg kg⁻¹ (11).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2B (12).

Subcutaneous rabbit, guinea pig (duration unspecified) 1.0 or 0.5 ml of a 2% solution in olive oil, respectively, 6 × wk⁻¹. Rabbits that survived >100 days developed papillomas in the bladder; guinea pigs did not survive long enough to develop papillomas (9).

Subcutaneous rat, rabbit, guinea pig (dose and duration unspecified). Papillomas developed in 1/2, 4/5 and 5/8 animals, respectively (9).

Irritancy

Dermal rabbit (24 hr) 10 mg caused mild irritation (11).

Dermal rabbit (24 hr) 500 mg caused mild irritation (13).

750 µg instilled in a rabbit eye (24 hr) caused severe irritation (14).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538, D3052, C3076, G46 with and without metabolic activation negative (15).

Escherichia coli WP2, WP2uvrA⁻ with and without metabolic activation negative (15).

Escherichia coli DNA repair test without metabolic activation positive (9).

Escherichia coli K12 prophage λ assay without metabolic activation positive (9).

In vitro primary rat hepatocytes unscheduled DNA synthesis negative (15).

In vitro Chinese hamster ovary cells with and without metabolic activation, sister chromatid exchanges and chromosomal aberrations positive (16).

In vitro V79 Chinese hamster cells did not induce single-strand breaks in DNA (9).

Other effects

Other adverse effects (human)

An increased incidence of bladder cancer has been seen in workers exposed to the compound as well as to other potentially carcinogenic compounds (9).

Any other adverse effects

Toxic effects include methaemoglobinaemia, reticulocytosis and anaemia in rat and methaemoglobinaemia in mice. The compound also produced keratosis and metaplasia in the epithelium of the bladder of rats (9).

Intragastric administration to rats caused cyanosis, spleen congestion and hypercellularity in bone marrow; oral administration caused changes in the bladder epithelium and a low incidence of papillomas (17).

Other comments

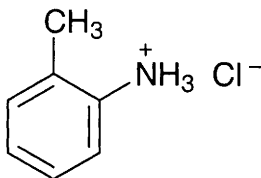
Reviews on human health effects, experimental toxicology, physico-chemical properties, epidemiology, workplace experience, ecotoxicology, environmental effects and exposure levels listed (18).

Autoignition temperature 480–482°C.

References

1. Fiedler, H. et al *Toxicol. Environ. Chem.* 1990, **28**, 167-188.
2. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
3. Bringmann, G. et al *Water Res.* 1980, **14**, 231-241.
4. Meinck, F. et al *Les eaux residuaires industrielles* 1970.
5. Alexander, M. et al *J. Agric. Food Chem.* 1966, **14**, 410.
6. Pitter, P. *Water Res.* 1976, **10**, 231-235.
7. Worne, H. E. *Tijdschrift van Het BECEWA*, Liege, Belgium.
8. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
9. *IARC Monograph* 1982, **27**, 155-175.
10. *US Public Health Service Public Health Bulletin* 1941, **271**, 49.
11. Smyth, H. F. *Am. Ind. Hyg. Assoc. J.* 1962, **23**, 95-112.
12. *IARC Monograph* 1987, **Suppl.** 7, 72.
13. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripavku* 1972, Prague, Czechoslovakia.
14. Marhold, J. V. *Prehled Prumyslove Toxikologie: Organicke Latky* 1986, Prague, Czechoslovakia.
15. Thompson, C. Z. et al *Environ. Mutagen.* 1983, **5**, 803-811.
16. Gulati, D. K. *Prog. Mutat. Res.* 1985, **5**, 413-426.
17. *Chemical Safety Data Sheets* 1991, **4b**, 221-224, The Royal Society of Chemistry, London, UK.
18. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T186 o-toluidine hydrochloride



C₇H₁₀ClN

Mol. Wt. 143.62

CAS Registry No. 636-21-5

Synonyms 2-methylbenzenamine, hydrochloride; o-methylaniline hydrochloride; o-toluidinium hydrochloride

EINECS No. 211-252-8

RTECS No. XU 7350000

Uses Dye intermediate used in the manufacture of textile dyes.

Physical properties

M. Pt. 215-217°C B. Pt. 242.2°C

Solubility Water: very soluble. Organic solvents: ethanol

Occupational exposure

UN No. 1708 HAZCHEM Code 3X Conveyance classification toxic substance

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 1100, 2951 mg kg⁻¹, respectively (1,2).

LD₅₀ intraperitoneal mouse, rat 113, 150 mg kg⁻¹, respectively (3).

Carcinogenicity and chronic effects

National Toxicology Program tested rats and mice via food. Positive evidence for carcinogenicity in ♂, ♀ rats and mice. The mean body weights of the dosed animals were lower than those of controls. Mortalities of ♂, ♀ rats were dose related and relatively high at the end of the study; mortalities of the mice were not affected by the compound. Haemangiosarcomas were induced at various sites in ♂ mice and hepatocellular carcinomas or adenomas were induced in ♀ mice. Sarcomas of the spleen and other organs were induced in ♂, ♀ rats; mesotheliomas of the abdominal cavity and scrotum were seen in ♂ and transitional-cell carcinomas in the urinary bladder in ♀. Administration of the compound also resulted in increased incidences of fibromas of the subcutaneous tissue in ♂ rats and fibroadenomas or adenomas of the mammary gland in ♀ rats (4).

Oral ♂, ♀ mice (102-103 wk) 1000 or 3000 mg kg⁻¹. No significant dose-related trend in mortality was seen, but statistically significant dose-related increases in tumour incidences were observed (5).

Oral ♂, ♀ rats (101-104 wk) 3000 or 6000 mg kg⁻¹. A significant dose-related trend in mortality was seen; all high-dose ♂ had died by 100 wk. Dose-related increases in tumour incidences were observed for several neoplasms (5).

Genotoxicity

Salmonella typhimurium positive (strains and metabolic activation unspecified) (6).

In vivo mice bone marrow cells sister chromatid exchanges positive, chromosomal aberrations, induction of micronuclei negative (7).

Drosophila melanogaster sex-linked recessive assay negative (8).

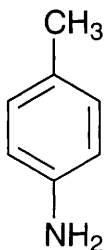
Other comments

Reviews on human health effects, epidemiology, workplace experience, experimental toxicology, environmental effects listed (9).

References

1. *Gig. Tr. Prof. Zabol.* 1981, **25**(8), 50.
2. *J. Pharmacol. Exp. Ther.* 1969, **167**, 223.
3. Sax, N. I. et al *Dangerous Properties of Industrial Materials* 8th ed., 1992, Van Nostrand Reinhold, New York, NY, USA.
4. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-153, NIEHS, Research Triangle Park, NC, USA.
5. *IARC Monograph* 1982, **27**, 155-175.
6. Ashby, J. et al *Mutat. Res.* 1991, **257**(3), 229-306.
7. McFee, A. F. et al *Environ. Mol. Mutagen.* 1989, **14**, 207-220.
8. Zimmering, S. et al *Environ. Mol. Mutagen.* 1989, **14**, 245-251.
9. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T187 *p*-toluidine



C₇H₉N

Mol. Wt. 107.16

CAS Registry No. 106-49-0

Synonyms 4-methylbenzenamine; 4-aminotoluene; 4-methylaniline; C.I. 37107; C.I. Azoic Coupling Component 107; *p*-tolylamine

EINECS No. 203-403-1

RTECS No. XU 3150000

Uses Manufacture of dyes and other organic chemicals. Reagent for lignin, nitrite and phloroglucinol.

Physical properties

M. Pt. 44-45°C **B. Pt.** 200-201°C **Flash point** 86°C **Specific gravity** 1.046 at 20°C with respect to water at 4°C **Partition coefficient** log *P*_{ow} 1.39 **Volatility** v.p. 1 mmHg at 42°C; v.den. 3.9

Solubility Water: soluble in 135 parts water. Organic solvents: acetone, diethyl ether, ethanol, methanol

Occupational exposure

US-TWA 2 ppm (8.8 mg m⁻³)

UN No. 1708 **HAZCHEM Code** 3X **Conveyance classification** toxic substance

Supply classification toxic, dangerous for the environment

Risk phrases Toxic by inhalation, in contact with skin and if swallowed – Danger of cumulative effects – Very toxic to aquatic organisms (R23/24/25, R33, R50)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – After contact with skin, wash immediately with plenty of water – Wear suitable protective clothing and gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S28, S36/37, S45, S61)

Ecotoxicity

Fish toxicity

Exposure to 5 ppm was non-toxic to bluegill sunfish, yellow perch and goldfish. Test conditions: temperature 30°C; dissolved oxygen 7.5 ppm; total hardness (soap method) 300 ppm; alkalinity 310 ppm (methyl orange); free carbon dioxide 5 ppm (1).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 4.27 ppm Microtox test (2).

Environmental fate

Degradation studies

Confirmed to be biodegradable (3).

ThOD 2.54 g O₂ g⁻¹; BOD₅ 1.44 g O₂ g⁻¹ (4).

Decomposition by a soil microflora in 4 days (5).

Activated sludge at 20°C with compound as sole carbon source COD 97.7%; 20 mg COD g dry inoculum⁻¹ hr⁻¹ (6).

Degradation by *Aerobacter* 500 mg l⁻¹ at 30°C; parent 100% ring disruption in 3 hr (7).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird, starling 56.2, 42.2 mg kg⁻¹, respectively (8).

LD₅₀ oral quail 237 mg kg⁻¹ (8).

LD₅₀ oral mouse, rat 330, 656 mg kg⁻¹, respectively (9,10).

LD₅₀ intraperitoneal mouse 50 mg kg⁻¹ (11).

Irritancy

Dermal rabbit (24 hr) 500 mg caused severe irritation; 100 mg instilled in rabbit eye caused severe irritation (10).

Dermal rabbit (24 hr) 500 mg caused mild irritation; 20 mg instilled in rabbit eye (24 hr) caused moderate irritation (12).

In rats, exposure to 640 mg m⁻³ caused nasal and eye irritation (duration unspecified) (13).

Sensitisation

Caused sensitisation in guinea pigs (14).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538, D3052, C3076, G46 with and without metabolic activation negative (15).

Escherichia coli WP2, WP2 *uvrA*⁻ with and without metabolic activation negative (15).

In vitro primary rat hepatocytes unscheduled DNA synthesis positive (15).

In vitro V79 Chinese hamster lung cells did not cause single-strand DNA breaks (16).

Other comments

Industrial hazards reviewed (17).

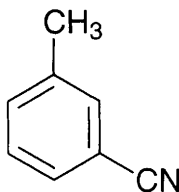
Reviews on human health effects, experimental toxicology, physico-chemical properties, workplace experience, ecotoxicology, epidemiology listed (18).

Autoignition temperature 482°C.

References

1. *The Toxicity of 3400 Chemicals to Fish* 1987, EPA560/6-87-002 P13 87-200-275, Washington, DC, USA.
2. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
3. *The list of the existing chemical substances tested on biodegradability by microorganisms or bioaccumulation in fish body* 1987, Chemicals Inspection and Testing Institute, Japan.
4. Meinck, F. et al *Les eaux residuaires industrielles* 1970.
5. Alexander, M. et al *J. Agric. Food Chem.* 1966, **14**, 410.
6. Pitter, P. *Water Res.* 1976, **10**, 231-235.
7. Worne, H. E. *Tijdschrift van Het BECEWA* Liege, Belgium.
8. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
9. *Gig. Tr. Prof. Zabol* 1981, **25**(8), 50.
10. *BIOFAX Industrial Bio-Test Laboratorie Inc. Data Sheets* 1973, 31-4.
11. *National Technical Information Service* AD691-490.
12. Marhold, J. V. *Šborník Výsledků Toxikologického Vysvětlení Latek A Přípravku* 1972, Prague, Czechoslovakia.
13. *Chemical Safety Data Sheets* 1991, **4b**, 225-227, The Royal Society of Chemistry, London, UK.
14. Kleniewska, D. et al *Dermatosen, Beruf, Umwelt* 1980, **28**, 11-13.
15. Thompson, C. Z. et al *Environ. Mutagen.* 1983, **5**, 803-811.
16. Zimmer, D. et al *Mutat. Res.* 1980, **77**, 371-326.
17. Ikeda, M. et al *Sumitomo Sangyo Eisei* 1985, **21**, 131-151.
18. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T188 *m*-tolunitrile



C_8H_7N

Mol. Wt. 117.15

CAS Registry No. 620-22-4

Synonyms 3-methylbenzonitrile; 3-cyanotoluene; *m*-tolyl nitrile

EINECS No. 210-631-5

RTECS No. XV 0525000

Physical properties

M. Pt. $-23^{\circ}C$ B. Pt. $99-101^{\circ}C$ at 20 mmHg Flash point $86^{\circ}C$ Specific gravity 0.976

Occupational exposure

UN No. 2810

Mammalian & avian toxicity

Acute data

LD₅₀ oral rabbit 4200 mg kg⁻¹ (1).

Irritancy

500 mg instilled into rabbit eye for 24 hr caused severe irritation (1).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535 with and without metabolic activation negative (2).

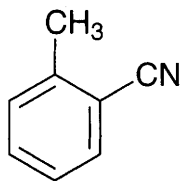
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Cyanides: maximum admissible concentration 50 µg l⁻¹ (3).

References

1. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
2. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, 11(Suppl. 12), 1-158.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T189 o-tolunitrile



C_8H_7N

Mol. Wt. 117.15

CAS Registry No. 529-19-1

Synonyms 2-methylbenzonitrile; 2-methylbenzenecarbonitrile; o-cyanotoluene; o-toluenecarbonitrile; o-tolyl nitrile

EINECS No. 208-451-7

RTECS No. XV 0600000

Physical properties

M. Pt. 13°C B. Pt. 205.2°C Flash point 84°C Specific gravity 0.9955 at 20°C with respect to water at 4°C

Partition coefficient $\log P_{ow}$ 2.21

Solubility Organic solvents: miscible with diethyl ether, ethanol

Ecotoxicity

Toxicity to other species

LD_{Lo} subcutaneous frog 1000 mg kg⁻¹ (1).

Mammalian & avian toxicity

Acute data

LD_{Lo} subcutaneous rabbit 600 mg kg⁻¹ (1).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535 with and without metabolic activation negative (2).

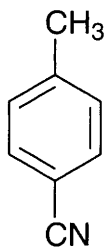
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Cyanides: maximum admissible concentration 50 µg l⁻¹ (3).

References

1. *Arch. Int. Pharmacodyn. Ther.* 1899, 5, 161.
2. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, 11 (Suppl.12), 1-158.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T190 *p*-tolunitrile



C_8H_7N

Mol. Wt. 117.15

CAS Registry No. 104-85-8

Synonyms 4-cyanotoluene; *p*-toluic nitrile; *p*-tolynitrile; 4-methylbenzonitrile; 4-methylcyanobenzene; *p*-toluenenitrile

EINECS No. 203-244-8

RTECS No. XV 0700000

Physical properties

M. Pt. 29.5°C **B. Pt.** 217.6°C **Flash point** 85°C **Specific gravity** 0.9785 at 30°C with respect to water at 4°C
Solubility Water: insoluble. Organic solvents: diethyl ether, ethanol

Ecotoxicity

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 4.56 ppm Microtox test (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird >100 mg kg⁻¹ (2).

LD₅₀ oral rat 4060 mg kg⁻¹ (3).

LD_{Lo} intraperitoneal mouse 512 mg kg⁻¹ (4).

LD_{Lo} subcutaneous rabbit 1080 mg kg⁻¹ (5).

Irritancy

Dermal rabbit (24 hr) 500 mg caused moderate irritation and 500 mg instilled in rabbit eye (24 hr) caused severe irritation (3).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535 with and without metabolic activation negative (6).

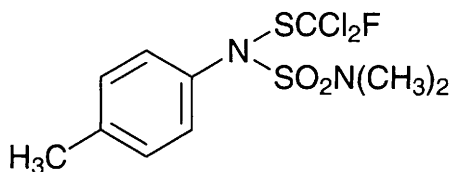
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Cyanides: maximum admissible concentration 50 µg l⁻¹ (7).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
2. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
3. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
4. *Summary Tables of Biological Tests* National Research Council Chemical-Biological Coordination Center, 1951, **3**, 129.
5. *Arch. Int. Pharmacodyn. Ther.* 1899, **5**, 161.
6. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-158.
7. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T191 tolylfluandid



C₁₀H₁₃Cl₂FN₂O₂S₂

Mol. Wt. 347.26

CAS Registry No. 731-27-1

Synonyms 1,1-dichloro-*N*-[(dimethylamino)sulfonyl]-1-fluoro-*N*-(4-methylphenyl)methanesulfenamide; *N*-[(dichlorofluoromethyl)thio]-*N,N'*-dimethyl-*N-p*-tolylsulfamide; BAY 5712a; Euparen M

EINECS No. 211-986-9

RTECS No. WO 6560000

Uses Fungicide. Acaricide.

Physical properties

M. Pt. 95-97°C **Partition coefficient** log *P*_{ow} 3.95 at 20°C (1) **Volatility** v.p. 9.78 × 10⁻⁸ mmHg at 45°C

Solubility Water: 0.9 mg l⁻¹ at room temperature. Organic solvents: benzene, methanol, xylene

Occupational exposure

Supply classification toxic, dangerous for the environment

Risk phrases Toxic by inhalation – Irritating to eyes and respiratory system – May cause sensitisation by skin contact – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R23, R36/37, R43, R50/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Avoid contact with the skin – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Wear suitable gloves – In case of insufficient ventilation, wear suitable respiratory equipment – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S24, S26, S37, S38, S45, S60, S61)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) goldfish 10 mg l⁻¹ (1).

LC₅₀ (96 hr) carp, roach 0.25-0.5 mg l⁻¹ (1).

LC₅₀ (96 hr) golden orfe 0.07-0.25 mg l⁻¹ (1).

Invertebrate toxicity

Non-toxic to bees (2).

Environmental fate

Abiotic removal

Hydrolysis at 22°C: t_{1/2} 12 days at pH 4, 29 hr at pH 7, <10 min at pH 9 (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral ♀ canary 1000 mg kg⁻¹ (1).

LD₅₀ oral rat, mouse >5000, >1000 mg kg⁻¹, respectively (1).

LD₅₀ oral guinea pig 250-500 mg kg⁻¹ (1).

LC₅₀ (1 hr) inhalation rat >0.408 mg l⁻¹ (1).

LD₅₀ percutaneous rat >5000 mg kg⁻¹ (1).

Carcinogenicity and chronic effects

In 2-yr feeding trials, no-effect level for rats was 300 mg kg⁻¹ diet (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (3).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (4).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (5).

WHO Toxicity Class Table 5 (6).

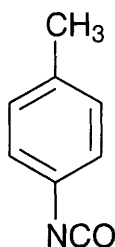
EPA Toxicity Class II (formation) (2).

ADI (JMPR) 0.1 mg kg⁻¹ body weight (2).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
4. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
5. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
6. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21

T192 *p*-tolyl isocyanate



C₈H₇NO

Mol. Wt. 133.15

CAS Registry No. 622-58-2

Synonyms 4-tolyl isocyanate; 1-isocyanato-4-methylbenzene; isocyanic acid, *p*-tolyl ester; *p*-methylphenyl isocyanate; *p*-toluene isocyanate

EINECS No. 210-743-4

Physical properties

B. Pt. 70-62°C at 10 mmHg Flash point 66°C Specific gravity 1.056

Occupational exposure

SE-LEVL 0.005 ppm

SE-CEIL 0.01 ppm

UK-LTEL MEL 0.02 mg m⁻³ (as NCO)

UK-STEL MEL 0.07 mg m⁻³ (as NCO)

Ecotoxicity

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 3.05 ppm Microtox test (1).

Other effects

Other adverse effects (human)

Recurrent exposure-related asthma and chronic pulmonary obstruction have been observed in isocyanate-exposed workers (2).

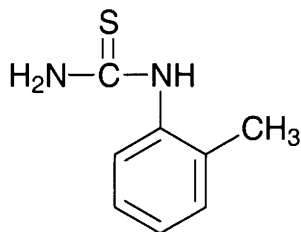
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Cyanides: maximum admissible concentration 50 µg l⁻¹ (3).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, 26(3), 361-431.
2. Baur, X. *Allergologie* 1986, 9(11), 487-496.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T193 o-tolylthiourea



C₈H₁₀N₂S

Mol. Wt. 166.25

CAS Registry No. 614-78-8

Synonyms (2-methylphenyl)thiourea; 2-thio-1-o-tolylurea; N-(o-tolyl)thiourea

EINECS No. 210-395-3

Physical properties

M. Pt. 151-152°C

Solubility Organic solvents: ethanol, hot diethyl ether

Mammalian & avian toxicity

Acute data

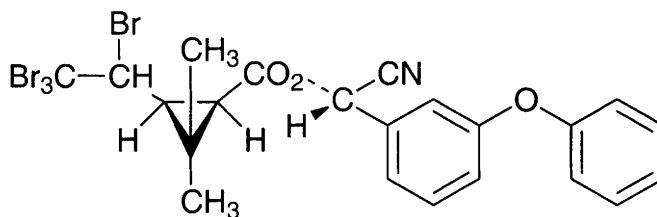
LD_{Lo} oral rat 5 mg kg⁻¹ (1).

LD₅₀ intraperitoneal mouse 150 mg kg⁻¹ (2).

References

1. *Natl. Acad. Sci., Natl. Res. Council Chem. Biol. Coord. Center Rev.* 1953, 5, 1.
2. *NTIS Report AD691-490*, Natl. Tech. Inf. Ser., Springfield, VA, USA

T194 tralomethrin



$C_{22}H_{19}Br_4NO_3$

Mol. Wt. 665.01

CAS Registry No. 66841-25-6

Synonyms (S)- α -cyano-3-phenoxycyano-3-phenylmethyl (1R,3S)-2,2-dimethyl-3-[(RS)-1,2,2,2-tetrabromoethyl]-cyclopropanecarboxylate; cyano(3-phenoxycyano-3-phenylmethyl) 2,2-dimethyl-3-[(1R,3S)-1,2,2,2-tetrabromoethyl]-cyclopropanecarboxylate; tralométhrine; Sag; Scout; Tracker; Tralate; Tralox

EINECS No. 266-493-1

Uses Pyrethroid insecticide.

Physical properties

M. Pt. 138-148°C **Flash point** 26°C **Specific gravity** 1.70 at 20°C **Partition coefficient** $\log P_{ow} > 5.0$

Volatility v.p. 1.3×10^{-3} mmHg at 25°C

Solubility Water: 70 mg kg⁻¹. Organic solvents: acetone, dichloromethane, toluene, xylene

Ecotoxicity

Invertebrate toxicity

LC₅₀ *Daphnia magna* 0.15 µg l⁻¹ (1).

LD₅₀ (contact) honeybee 0.12 µg bee⁻¹. Low LD₅₀ and LC₅₀ values under laboratory conditions do not represent significant hazard to bees in normal feed use (2).

Environmental fate

Adsorption and retention

Strongly adsorbed in soil, DT₅₀ 64-84 days. K_D 197-8784, K_{oc} 43796-675667. Highly immobile in soils from sandy to clay loam (2).

Mammalian & avian toxicity

Acute data

LD₅₀ rats 99-3000 mg kg⁻¹, depending on carrier used (2).

LC₅₀ (4 hr) rats >0.286 mg l⁻¹ air (2).

LD₅₀ dermal rabbits >2000 mg kg⁻¹ (2).

Carcinogenicity and chronic effects

No-observed-effect limit (2 yr) rats 0.75 mg kg⁻¹ daily in diet, mice 3 mg kg⁻¹ daily in diet (2).

Teratogenicity and reproductive effects

Not teratogenic in rats or rabbits (2).

Metabolism and toxicokinetics

Following oral administration to rats, tralomethrin is rapidly debrominated to form deltamethrin, which is then hydroxylated and undergoes ester cleavage reactions, yielding a series of alcohols and carboxylic acids and their glucuronide, glycine, and sulfate conjugates. The cyano fragment is retained for several days in the stomach and skin (3).

Irritancy

Mild eye irritant in rabbits (2).

Sensitisation

Moderate skin irritant in rabbits (2).

Genotoxicity

Not mutagenic in rats or rabbits (2).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (4).

Included in Schedule 6 (Release into Land: Prescribed Substances) of Statutory Instrument No. 472, 1991 (5).

The US Federal Food, Drug, and Cosmetic Act has established a tolerance of 0.05 ppm for combined residues of tralomethrin and its metabolite (S)- α -cyano-3-phenoxybenzyl (1R,3R)-3-(2,2-dibromovinyl)-2,2-dimethylcyclopropanecarboxylate in or on soybeans (6).

WHO Toxicity Class II (7).

EPA Toxicity Class II (formulation) (2).

Acceptable daily intake $0.0075 \text{ mg kg}^{-1}$ body weight (2).

Other comments

In the mouse, intracerebrally administered tralomethrin may be activated by debromination in the brain (3).

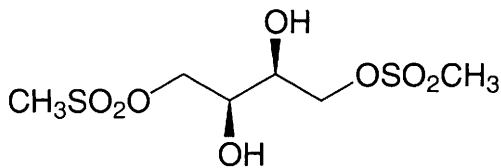
Tralomethrin undergoes debromination to form deltamethrin following topical administration to house flies, feeding to cabbage looper larvae, or incubation with house fly homogenates and cockroach nerve cords.

Following debromination, an esterase(s) in house fly homogenate hydrolyses deltamethrin (8).

References

1. Mokry, L. E. et al *Environ. Toxicol. Chem.* 1990, 9(8) 1045-1051.
2. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
3. Cole, L. M. et al *J. Agric. Food Chem.* 1982, 30(4), 631-636.
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
5. *S.I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
6. *Fed. Regist.* 1987, 52(116), 23039, 17 June 1997.
7. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
8. Ruza, L. O. et al *Pestic. Biochem. Physiol.* 1981, 15(2), 137-142

T195 treosulfan



$C_6H_{14}O_8S_2$

Mol. Wt. 278.30

CAS Registry No. 299-75-2

Synonyms L-threitol (2S,3S)-1,4-dimethanesulfonate; 1,2,3,4-butanetetrol, 1,4-dimethanesulfonate, [S-(R,R)]-; Threosulphan; dihydroxybusulfan; NSC-39069

EINECS No. 206-081-0

RTECS No. XO 8500000

Uses Antineoplastic agent for the treatment of ovarian cancer.

Occurrence Not known to occur naturally (1).

Physical properties

M. Pt. 102°C

Solubility Water: soluble in 14 parts water. Organic solvents: acetone, chloroform, ethanol

Mammalian & avian toxicity

Acute data

Anorexia and weight loss, depression of bone-marrow activity, reticulocytopenia and leucopenia were seen in dogs and monkeys given the LD₅₀ dose (1).

Sub-acute and sub-chronic data

LD₅₀ (5 day) oral rat 462-963 mg kg⁻¹ day⁻¹ (1).

LD₅₀ (13 day) oral monkey 222-444 mg kg⁻¹ day⁻¹ (1).

LD₅₀ (18 day) intravenous dog 111 mg kg⁻¹ day⁻¹ (1).

LD₅₀ (14 day) intravenous monkey 111 mg kg⁻¹ day⁻¹ (1).

Anorexia and weight loss, depression of bone-marrow activity, reticulocytopenia and leucopenia were seen in dogs and monkeys given the LD₅₀ dose (1).

Carcinogenicity and chronic effects

Sufficient evidence for carcinogenicity to humans and animals, IARC classification group 1 (2).

Genotoxicity

Salmonella typhimurium TA100, TA1535 positive (metabolic activation unspecified) (3).

In vivo mice bone marrow cells micronucleus test positive (4,5).

In vivo mice peripheral blood cells micronucleus test positive (5).

Predicted to be genotoxic, based on its structure (6).

Induced chromosomal aberrations in seeds of *Allium cepa*, *Hordeum sativum*, *Nigella damascena* and *Vicia faba* (1).

Other effects

Other adverse effects (human)

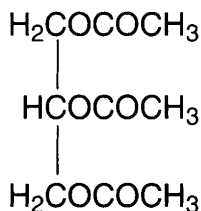
13/553 patients with ovarian cancer treated only with treosulfan developed acute non-lymphocytic leukaemia; the expected number of cases was <0.1 (7).

Nausea and vomiting occur in ~20% of patients and platelet and leucocyte counts drop within 4 wk of the start of oral therapy; blood cell counts return to normal in a month (1).

References

1. IARC Monograph 1981, **26**, 341-349.
2. IARC Monograph 1987, **Suppl. 7**, 73.
3. Zeiger, E. et al *Environ. Mol. Mutagen.* 1989, **13**(4), 343-346.
4. Shelvy, M. D. et al *Environ. Mol. Mutagen.* 1989, **13**(4), 339-342.
5. Gulati, D. K. et al *Mutat. Res.* 1990, **234**(3-4), 135-139.
6. Shelby, M. D. *Mutat. Res.* 1988, **204**(1), 3-15.
7. Pedersen-Bjergaard, J. et al *Ann. Intern. Med.* 1985, **103**, 195-200

T196 triacetin



C₉H₁₄O₆

Mol. Wt. 218.21

CAS Registry No. 102-76-1

Synonyms glycerin triacetate; glycerol triacetate; glyceryl triacetate; triacetyl glycerin; 1,2,3-propanetriol triacetate

EINECS No. 203-051-9

RTECS No. AK 3675000

Uses Fixative in perfumes. Solvent for dyes. Used as a fungistat in food and cosmetic industries.

Physical properties

M. Pt. -78°C **B. Pt.** 258-260°C **Flash point** 138°C **Specific gravity** 1.1596 at 20°C with respect to water at 4°C **Volatility** v.den. 7.5

Solubility Organic solvents: slightly soluble in carbon disulfide, miscible with chloroform, diethyl ether, ethanol

Ecotoxicity

Toxicity to other species

Complete narcosis in *Rana temporaria* with 5000 mg l⁻¹ (observed), 19,000 mg l⁻¹ (predicted) (1).

LD_{Lo} oral frog 150 mg kg⁻¹ (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 3000 mg kg⁻¹ (3).

LD₅₀ oral mouse 1400 mg kg⁻¹ (4).

LD₅₀ subcutaneous mouse, rat 2300-2800 mg kg⁻¹ (5).

LD₅₀ intraperitoneal rat 2100 mg kg⁻¹ (2).

LD₅₀ intraperitoneal mouse 1400 mg kg⁻¹ (4).

LD₅₀ intravenous rabbit, dog 750 and 1500 mg kg⁻¹, respectively (2).

Intravenous studies showed lowest lethal values of 1.5-2.0 ml kg⁻¹ for dogs, 0.75 ml kg⁻¹ for rabbits and a no-effect dose of 0.5 ml kg⁻¹ for rabbits. Animals near death exhibited muscular tremors, convulsions and severe dyspnea 2-22 min after injection (6).

Sub-acute and sub-chronic data

Inhalation rat (13 wk) 6 hr day⁻¹, 5 day wk⁻¹ produced no symptoms or histopathological effects (6).

Irritancy

Not classed as an irritant following instillation into the eye of a rabbit (7).

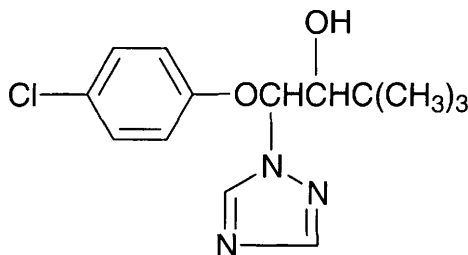
Non-irritant when absorbed through guinea pig skin (6).

Sensitisation

Not a skin sensitiser (6).

References

1. Lipnick, R. L. *ASTM Spec. Tech. Publ.* 1988, **1007**(Aquat. Toxicol. Environ. Fate), 468-489.
2. *Food Cosmet. Toxicol.* 1978, **16**, 637.
3. *AMA Arch. Ind. Health* 1960, **21**, 28.
4. *Fed. Proc., Fed. Am. Soc. Exp. Biol.* 1963, **22**, 368.
5. *Proc. Soc. Exp. Biol. Med.* 1941, **46**, 26.
6. Clayton, G. D. et al (Eds.) *Patty's Industrial Hygiene and Toxicology* 3rd ed., 1981, **2A**, John Wiley & Sons, New York, NY, USA.
7. Jacobs, G. A. et al *Food Chem. Toxicol.* 1989, **27**(4), 255-258

T197 triadimenol

C₁₄H₁₈ClN₃O₂

Mol. Wt. 295.77

CAS Registry No. 55219-65-3

Synonyms Baytan; β-(4-chlorophenoxy)-α-(1,1-dimethylethyl)-1*H*-1,2,4-triazole-1-ethanol;
1-(4-chlorophenoxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)butan-2-ol; Spinnaker; Summit

EINECS No. 259-537-6

RTECS No. KK 2200000

Uses Fungicide.

Physical properties

M. Pt. 133.5°C (1*RS*,2*SR*); 138.2°C (1*RS*,2*RS*) **Partition coefficient** log *P*_{ow} 3.28 (1*RS*,2*RS*); 3.08 (1*RS*,2*SR*) both at 25°C **Volatility** v.p. <1 × 10⁻⁵ mmHg at 20°C

Solubility Water: 33 mg l⁻¹ (1*RS*,2*RS*); 62 mg l⁻¹ (1*RS*,2*SR*) both at 20°C. Organic solvents: acetone, dichloromethane, ethanol, hexane, isopropyl alcohol, toluene

Ecotoxicity**Fish toxicity**

LC₅₀ (96 hr) bluegill sunfish, golden orfe, goldfish, rainbow trout 10-50 mg l⁻¹ (1,2).

Invertebrate toxicity

Non-toxic to honeybees (2).

Environmental fate

Degradation studies

$t_{1/2}$ 110-375 days in sandy loam, 240-270 days in loam (1).

Stable to hydrolysis at 22°C, with $t_{1/2}$ >1 yr (1).

Undergoes hydrolytic cleavage leading to the formation of 4-chlorophenol. Metabolism of the individual enantiomers proceeds at different rates (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral Japanese quail, hen, canaries 1750-2500, >2000, >1000 mg kg⁻¹, respectively (1).

LC₅₀ (4 hr) inhalation rat >0.45 mg l⁻¹ (1).

LD₅₀ oral rat, mouse 700-1200, 1300 mg kg⁻¹, respectively (1,2).

LD₅₀ oral ♂ dog >500 mg kg⁻¹ (1).

LD₅₀ dermal rat >5000 mg kg⁻¹ (2).

Sub-acute and sub-chronic data

Oral rat, dog (3 month) no-adverse-effect level 600 mg kg⁻¹ diet (1).

Carcinogenicity and chronic effects

Oral rat, mouse (2 yr) no-adverse-effect level for rats 50 mg kg⁻¹ diet, and for mice 125 mg kg⁻¹ diet (1).

Metabolism and toxicokinetics

Following oral administration to rats, excreted in approximately equal proportions in the urine and faeces.

Metabolism principally involves hydroxylation and oxidation (1).

Irritancy

Non-irritating to rabbit eyes and skin (1).

Sensitisation

Non-sensitising to guinea pig skin (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (4).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (5).

EEC maximum residue limits: pineapples 2 ppm; other fruits, cucurbits 1 ppm; grapes, wheat 0.1 ppm (1).

Log P_{ow} value exceeds The European Community recommended level 3.0 (6th and 7th amendments) (6).

WHO Toxicity Class III (7).

EPA Toxicity Class III (formulation) (2).

ADI (JMPR) 0.05 mg kg⁻¹ (2).

Other comments

Active metabolite of triadimefon (8).

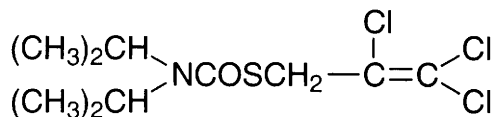
Reported to have no embryotoxic, teratogenic or mutagenic activity (1).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
3. Clark, T. et al *Proc. Br. Crop Prot. Conf. - Pests Dis.* 1986, 475.
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.

5. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations 1991*, HMSO, London, UK.
6. 1967 Directive on Classification, Packaging and Labelling of Dangerous Substances 67/548/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
7. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification 1998-1999* WHO/PCS/98.21.
8. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA

T198 tri-allate



$\text{C}_{10}\text{H}_{16}\text{Cl}_3\text{NOS}$

Mol. Wt. 304.67

CAS Registry No. 2303-17-5

Synonyms S-2,3,3-trichloroallyl di-isopropyl(thiocarbamate); S-(2,3,3-trichloro-2-propenyl) bis(1-methylethyl)carbamothioate; S-2,3,3-trichloroallyl di-isopropylthiocarbamate; Avadex BW; CP 23426

EINECS No. 218-962-7

RTECS No. EZ 8575000

Uses Herbicide.

Physical properties

M. Pt. 29-30°C **B. Pt.** 117°C at 0.0003 mmHg **Flash point** 95°C (open cup); 90°C (closed cup)

Specific gravity 1.273 at 25°C **Volatility** v.p. 1.2×10^{-4} mmHg at 25°C

Solubility Water: 4 mg l⁻¹ at 25°C. Organic solvents: acetone, benzene, diethyl ether, ethanol, heptane

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed (R22)

Safety phrases Keep out of reach of children (if sold to general public) (S2)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) rainbow trout, bluegill sunfish 1.2, 1.3 mg l⁻¹, respectively (1).

Invertebrate toxicity

LC₅₀ (48 hr) *Daphnia magna* 0.43 mg l⁻¹ (1).

Non-toxic to bees (2).

Environmental fate

Degradation studies

It is hydrolytically cleaved in soil, with the formation of dialkylamine, carbon dioxide and mercaptan moieties. The latter is transformed via sulfhydryl group exchange into the corresponding alcohol (1).

t_{1/2} in soil with medium moisture levels was 28.1 days in sandy loam and 25.9 days in loamy sand (10 µg g⁻¹ applied) (3).

Abiotic removal

Stable to light, decomposition temperature >200°C (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral bobwhite quail >2251 mg kg⁻¹ (1).
LD₅₀ oral rat, mouse 1100, 930 mg kg⁻¹, respectively (1,4).
LD₅₀ percutaneous rabbit 8200 mg kg⁻¹ (1).
LC_{Lo} (4 hr) inhalation cat 400 mg m⁻³ (4).
LD₅₀ dermal rabbit 2225 mg kg⁻¹ (5).

Sub-acute and sub-chronic data

LC₅₀ (8 day) oral mallard duck, bobwhite quail >5000 mg kg⁻¹ diet (1).
Inhalation of saturated air for 12 hr had no harmful effects on rats (1).
Oral hen single dose of 312.5-2500 mg kg⁻¹ on days 1 and 21 then killed on day 42, 25-300 mg kg⁻¹ day⁻¹ for 90 days, or single dose of 2500 mg kg⁻¹ and killed 24 hr later. Hens given daily doses of 300 mg kg⁻¹ became moribund after 30 days, but histological examination revealed no lesions characteristic of organophosphorus-induced delayed neurotoxicity (6).

Carcinogenicity and chronic effects

In 2-yr feeding trials no-effect level for rats was 50 mg kg⁻¹ diet and for mice was 20 mg kg⁻¹ diet (1).
In 1-yr feeding trials no-effect level for dogs was 2.5 mg kg⁻¹ diet (1).

Irritancy

Highly irritating to skin and slightly irritating to eyes of rabbits (1).

Genotoxicity

Salmonella typhimurium TA100, TA1535 with and without metabolic activation positive (7).
Bacillus subtilis TKJ6321 with and without metabolic activation positive, TKJ5211 negative (7).
Escherichia coli DNA-damaging activity, mitotic recombination negative (8).
Escherichia coli moderate mutagenic activity (no further details given) (8).
Saccharomyces cerevisiae DNA-damaging activity, mitotic recombination negative (8).
Saccharomyces cerevisiae moderate mutagenic activity (no further details given) (8).
A CASE study predicted the compound to be mutagenic (9).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (10).
Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (11).
WHO Toxicity Class III (12).
EPA Toxicity Class III (formulation) (2).
EEC MRL – fruit and vegetables 0.1 ppm (1).

Other comments

Metabolic pathways reviewed (13).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
3. Sing, G. et al *Environ. Pollut.* 1990, **66**(3), 253-262.
4. *Gig. Sanit.* 1968, **33**(7), 37.
5. Frear, E. H. (Ed.) *Pesticide Index* State College, PA, College Science Publications, 1969.
6. Lapadula, D. M. et al *Appl. Toxicol.* 1990, **14**(1), 191-198.
7. Shiau, S. Y. et al *J. Agric. Food Chem.* 1981, **29**(21), 268-271.
8. Emnova, E. E. et al *Egetika (Moscow)* 1986, **22**(10), 2416-2422 (Russ.) (*Chem. Abstr.* **106**, 80111g).
9. Klopman, G. et al *Mutat. Res.* 1990, **228**(1), 1-50.

10. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
11. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
12. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
13. Roberts, T. R. et al (Eds.) *Metabolic Pathways of Agrochemicals. Part 1: Herbicides and Plant Growth Regulators* 1998, The Royal Society of Chemistry, Cambridge, UK

T199 triallylamine



C₉H₁₅N

Mol. Wt. 137.22

CAS Registry No. 102-70-5

Synonyms *N,N*-di-2-propenyl-2-propen-1-amine; tri-*N*-allylamine

EINECS No. 203-048-2

RTECS No. XX 5950000

Uses Corrosion inhibitor. Catalyst. Organic synthesis.

Physical properties

M. Pt. <-70°C **B. Pt.** 150-151°C **Flash point** 30°C (open cup) **Specific gravity** 0.800 at 20°C with respect to water at 4°C **Partition coefficient** log *P*_{ow} 2.59 **Volatility** v.den. 4.73

Solubility Water: 2500 mg l⁻¹. Organic solvents: acetone, benzene, diethyl ether, ethanol

Occupational exposure

UN No. 2610 **HAZCHEM Code** 3Y **Conveyance classification** flammable liquid, corrosive

Environmental fate

Degradation studies

Degradation by *Aerobacter* 200 mg l⁻¹ at 30°C; 47% in 120 hr by parent strain, 100% in 22 hr by mutant strain (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 490, 1030 mg kg⁻¹, respectively (2,3).

LC₅₀ (4 hr) inhalation rat 2800 mg m⁻³ (4).

LD₅₀ dermal rabbit 400 mg kg⁻¹ (2).

LD₅₀ intraperitoneal mouse 190 mg kg⁻¹ (3).

Sub-acute and sub-chronic data

Inhalation rat 100 or 200 ppm 7 hr day⁻¹ for 50 days caused reduced body weight gain, changes in liver and kidney weight and some fatalities (5).

Irritancy

Dermal rabbit (24 hr) 10 mg caused severe irritation (2).

50 mg instilled into rabbit eye for 20 sec caused mild irritation (3).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (6).

Other comments

Physical properties, use, toxicity and safety precautions reviewed (7).

References

1. Worne, H. E. *Tijdschrift van het BECEWA* Liege, Belgium.
2. *Am. Ind. Hyg. Assoc. J.* 1962, **23**, 95.
3. *Arch. Environ. Health* 1960, **1**, 343.
4. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
5. *Patty's Industrial Hygiene and Toxicology* 2nd ed., 1963, **2**, 2057, John Wiley & Sons, New York, NY, USA.
6. Zeiger, E. et al *Environ. Mutagen.* 1987, **9**(Suppl. 9), 1-109.
7. *Chemical Safety Data Sheets* 1992, **5**, 246-248, The Royal Society of Chemistry, London, UK

T200 triallyl borate



$\text{C}_9\text{H}_{15}\text{BO}_3$

Mol. Wt. 182.03

CAS Registry No. 1693-71-6

Synonyms tris(2-propenyl) borate

EINECS No. 216-897-9

Physical properties

B. Pt. 177.3-179.3°C Specific gravity 0.9205 at 20°C

Occupational exposure

UN No. 2609 HAZCHEM Code 2X Conveyance classification toxic substance

Mammalian & avian toxicity

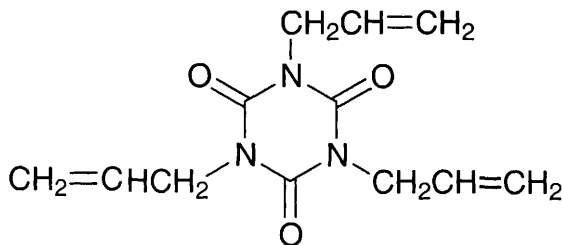
Acute data

LD₅₀ oral mouse 1800 mg kg⁻¹ (1).

References

1. U.S. Borax and Chemical Co. *Report* 1958, **32**

T201 triallyl isocyanurate



$C_{12}H_{15}N_3O_3$

Mol. Wt. 249.27

CAS Registry No. 1025-15-6

Synonyms 1,3,5-tris(2-propenyl)-1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione; triallyl-1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione

EINECS No. 213-834-7

RTECS No. XZ 1915000

Physical properties

M. Pt. 27°C **B. Pt.** 149-152°C at 4 mmHg **Flash point** >110°C **Specific gravity** 1.159

Solubility Water: <1 g l⁻¹ at 20°C. Organic solvents: acetone, dimethyl sulfoxide, ethanol

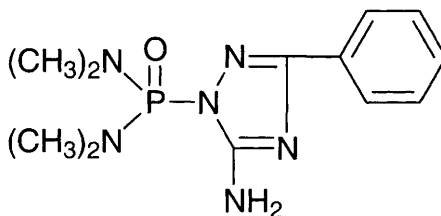
Genotoxicity

In vitro Chinese hamster ovary cells sister chromatid exchanges, chromosomal aberrations with and without metabolic activation negative (1).

References

1. Loveday, K. S. et al *Environ. Mol. Mutagen.* 1990, **16**(4), 272-303

T202 triamiphos



$C_{12}H_{19}N_6OP$

Mol. Wt. 294.30

CAS Registry No. 1031-47-6

Synonyms 5-amino-1-bis(dimethylamido)phosphoryl-3-phenyl-1,2,4-triazole; 5-amino-3-phenyl-1,2,4-triazole-1-yl-*N,N,N',N'*-tetramethylphosphodiamide; bis(dimethylamino)-3-amino-5-phenyltriazolyl phosphine oxide; Niagara 5943; Wepsin; WP 155

RTECS No. TA 1400000

Uses Superseded fungicide.

Physical properties

M. Pt. 167-168°C

Solubility Water: 250 mg l⁻¹ at 20°C. Organic solvents: benzene, chloroform, diethyl ether, ethanol

Occupational exposure

Supply classification very toxic

Risk phrases Very toxic in contact with skin and if swallowed (R27/28)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Do not breathe dust – After contact with skin, wash immediately with plenty of water – Wear suitable protective clothing and gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S22, S28, S36/37, S45)

Ecotoxicity

Invertebrate toxicity

Honeybees tolerate 10 mg kg⁻¹ diet (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 10, 20 mg kg⁻¹, respectively (1-3).

LD₅₀ dermal rat 48 mg kg⁻¹, rabbit 1500-3000 mg kg⁻¹ (1,4,5).

LD₅₀ intraperitoneal rat 15 mg kg⁻¹ (6).

Teratogenicity and reproductive effects

Oral rat, lowest toxic dose 1.3 mg kg⁻¹ day⁻¹ over several generations (affecting hepatobiliary system, endocrine system and congenital system). Doses of 6.6 mg kg⁻¹ day⁻¹ affected the blood and lymphatic systems (7).

Metabolism and toxicokinetics

In mammals absorbed through the skin, lungs and gastro-intestinal tract (5).

Genotoxicity

Saccharomyces cerevisiae D4 and *Aspergillus nidulans* mitotic gene conversion negative (8).

Other effects

Any other adverse effects

Cholinesterase inhibitor (5).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (9).

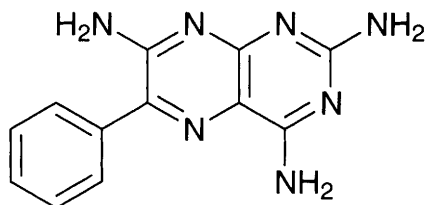
Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (10).

References

1. *The Pesticide Manual* 6th ed., 1979, 525, British Crop Protection Council, Farnham, UK.
2. *World Rev. Pest Control* 1970, **9**, 119.
3. *USDA Information Memorandum* 1966, **20**, 27.
4. *World Rev. Pest Control* 1970, **9**, 119.
5. *Guide to Chemicals Used in Crop Protection* 1973, **6**, 73, Information Canada, Ottawa, Canada.
6. *Eur. J. Pharmacol.* 1971, **16**, 361.
7. *Toxicology* 1974, **2**, 327.
8. de Bertaldi, M. et al *Environ. Mutagen.* 1980, **2**, 359-370.

9. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
10. S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations 1991, HMSO, London, UK

T203 triamterene



$C_{12}H_{11}N_7$

Mol. Wt. 253.27

CAS Registry No. 396-01-0

Synonyms Ademine; Diren; Dyrenium; Jatropur; Noridyl; 6-phenyl-2,4,7-pteridinetriamine; Pterofen; Tatevil; 2,4,7-triamino-6-phenylpteridine; Triampur; Tri-span; Triteren; Urocaudal

EINECS No. 206-904-3

RTECS No. UO 3470000

Uses Organic synthesis. Diuretic. Anti-malarial agent.

Physical properties

M. Pt. 316°C

Solubility Water: <1 g l⁻¹ at 18°C. Organic solvents: chloroform, diethyl ether, dimethylformamide, dimethyl sulfoxide, formic acid

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 290, 400 mg kg⁻¹, respectively (1,2).

LD₅₀ subcutaneous mouse 620 mg kg⁻¹ (3).

LD₅₀ intraperitoneal mouse 250 mg kg⁻¹ (3).

Carcinogenicity and chronic effects

National Toxicology Program tested rats and mice via feed. Some evidence of carcinogenicity was reported in ♂ and ♀ mice, equivocal results in ♂ rats, negative results in ♀ rats (4).

Metabolism and toxicokinetics

In humans, absorption from gastro-intestinal tract is enhanced by fat in the diet, and improved while fasting (5).

Rapidly absorbed from the gastro-intestinal tract. Excreted in the urine with peak renal excretion in 1-2 hr. 10-88% of oral dose may be recovered in the urine within 24 hr. In plasma ~67% is bound to protein (6).

Metabolites include hydroxytriamterene and hydroxytriamterene sulfuric acid (7).

Irritancy

Irritating to the eyes, skin, mucous membranes and upper respiratory tract (8).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1538 with and without metabolic activation negative (9).

Other effects

Other adverse effects (human)

Following administration of a single 100 mg dose, triamterene crystals and casts seen in the urine within 2-11 hr. Animal studies showed that crystallisation and cast formation occurred in the medullary and papillary collecting ducts in the rat kidney. These findings may account for nephrotoxicity of triamterene (10).

Severe hypokalaemia can occur in patients with impaired renal function or in those receiving supplementary potassium. Triamterene has also been reported to cause photosensitivity reactions, increased uric acid concentrations and blood dyscrasias. Nephrolithiasis may occur in susceptible patients, and megaloblastic anaemia has been reported in patients with depleted folic acid stores, such as those with hepatic cirrhosis. Reversible renal failure, due either to acute intestinal nephritis or to an interaction with non-steroidal anti-inflammatory drugs has occurred (11).

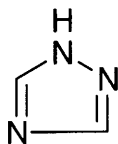
Most common side-effects are nausea, vomiting, leg cramps and dizziness. Slight-to-moderate azotemia is relatively common. This does not appear to be directly related to electrolyte and water imbalance and is reversible (6).

Triamterene and its metabolites inhibited dihydrofolate reductase activity of human leukocytes (7).

References

1. French Demande Patent Doc. 2314719.
2. Gekkan Yakuji 1979, 21, 775.
3. *Drugs in Japan: Ethical Drugs* 6th ed., 1982, 519, Jakugyo Jiho Co. Tokyo, Japan.
4. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-420, NIEHS, Research Triangle Park, NC, USA.
5. Williams, R. L. et al *Pharm. Res.* 1987, 4(4), 348-352.
6. Goodman, L. S. et al (Eds.) *The Pharmacological Basis of Therapeutics* 5th ed., 1975, 838, MacMillan, NY, USA.
7. Sehalhorn, A. et al *Arzneim.-Forsch* 1979, 29(9), 1409.
8. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, 2, 3389, Sigma-Aldrich, Milwaukee, WI, USA.
9. Mortelmans, K. et al *Environ. Mutagen.* 1986, 8(Suppl. 6), 1-119.
10. Fairley, K. F. et al *Clin. Nephrol.* 1986, 26(4), 169-173.
11. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK

T204 1,2,4-triazole



$C_2H_3N_3$

Mol. Wt. 69.07

CAS Registry No. 288-88-0

Synonyms pyrroldiazole; 1H-1,2,4-triazole

EINECS No. 206-022-9

RTECS No. XZ 3806000

Uses Organic synthesis.

Physical properties

M. Pt. 119-121°C B. Pt. 260°C

Solubility Water: soluble. Organic solvents: benzene, ethanol

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed – Irritating to the eyes – Possible risk of harm to the unborn child (R22, R36, R63)

Safety phrases Keep out of reach of children (if sold to general public) – Wear suitable protective clothing and gloves (S2, S36/37)

Ecotoxicity

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 5200 ppm Microtox test (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral quail >310 mg kg⁻¹ (2).

LD₅₀ oral rat, mouse 1350-1750 mg kg⁻¹ (3).

Sub-acute and sub-chronic data

Oral rat, mouse 0.2 mg kg⁻¹ day⁻¹ for 6 months caused no toxic effects (3).

Irritancy

Dermal rabbit 25% solution caused irritation and a 12% solution instilled into rabbit eye caused irritation (exposure unspecified) (3).

Legislation

Recommended maximum permissible concentration in water reservoirs 4 mg l⁻¹ (3).

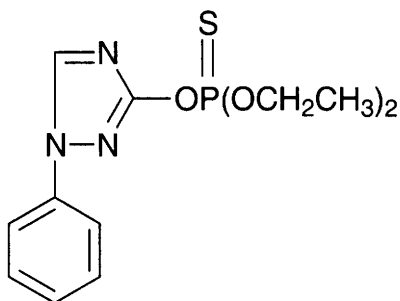
Other comments

Reported not to have teratogenic or genotoxic effects (4).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
2. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
3. Saratikov, A. S. et al *Gig. Sanit.* 1986, (11), 65-66 (Russ.) (*Chem. Abstr.* **106**, 97511k).
4. Rakhmatov, R. M. et al *Gig. Sanit.* 1991, (2), 30-31 (Russ.) (*Chem. Abstr.* **115**, 108000g)

T205 triazophos



$C_{12}H_{16}N_3O_3PS$

Mol. Wt. 313.32

CAS Registry No. 24017-47-8

Synonyms *O,O*-diethyl *O*-(1-phenyl-1*H*-1,2,4-triazol-3-yl) phosphorothioate; Hostathion; Hoe 2960; 1-phenyl-1,2,4-triazolyl-3-(*O,O*-diethyl thionophosphate)

EINECS No. 245-986-5

RTECS No. TF 5635000

Uses Insecticide. Nematocide. Acaricide.

Physical properties

M. Pt. 2-5°C **B. Pt.** decomposes on distillation **Flash point** 135°C (closed cup); 193°C (open cup)

Specific gravity 1.247 at 20°C with respect to water at 4°C **Partition coefficient** $\log P_{ow}$ 3.34

Volatility v.p. 2.9×10^{-3} mmHg at 30°C

Solubility Water: 30-40 mg l⁻¹ at 20°C. Organic solvents: acetone, ethanol, ethyl acetate, hexane, toluene

Occupational exposure

Supply classification toxic

Risk phrases Toxic in contact with skin and if swallowed (R24/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Do not breathe vapour – Wear suitable protective clothing and gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S23, S36/37, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) carp, goldfish, golden orfe 5.6-11 mg l⁻¹ (1).

Invertebrate toxicity

Toxic to honeybees (2).

Environmental fate

Degradation studies

Degradation t_{1/2} 18 and 87 days in two different German soils (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral Japanese quail 4.2-27.1 mg kg⁻¹ (1).

LD₅₀ oral rat 57-68 mg kg⁻¹ (1,4).

LD₅₀ oral dog >320 mg kg⁻¹ (5).

LC₅₀ (4 hr) inhalation rat 280 mg m⁻³ (6).

LD₅₀ dermal rat 1100 mg kg⁻¹ (5).
LD₅₀ intraperitoneal rat 110 mg kg⁻¹ (4).

Carcinogenicity and chronic effects

Oral rat, dog (2 yr) 1 mg kg⁻¹ diet for rats, 0.3 mg kg⁻¹ diet for dogs caused no adverse effects except inhibition of blood serum cholinesterase activity (1).

Metabolism and toxicokinetics

Following oral administration to rats, triazofos was rapidly metabolised, with 90% of the dose being excreted within 72 hr. The metabolites were 3,4,5-tribromo-*N*- α -dimethylpyrazole-1-acetamide, 3,4,5-tribromo- α -methylpyrazole-1-acetic acid and 3,4-dibromo- α -methylpyrazole-1-acetic acid (3).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (7).

Drosophila melanogaster sex-linked recessive lethal assay positive (8).

In vivo mouse micronucleous assay negative (9).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 μ g l⁻¹ (10).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (11).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (12).

WHO Toxicity Class Ib (13).

ADI (JMPR) 0.001 mg kg⁻¹ body weight (2).

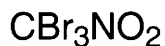
Other comments

In the cotton plant the metabolite 1-phenyl-3-hydroxy-1,2,4-triazole is formed (1).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
3. Menzie, C. M. *Metabolism of Pesticides – Update III* 1980, 543, Special Scientific Report – Wildlife No. 232, US Dept. Interior, Fish and Wildlife, Washington, DC, USA.
4. *Farm Chemicals Handbook* 1991, C166, Meister Publishing, Willoughby, OH, USA.
5. *Guide to Chemicals Used in Crop Protection*. 1973, 6, 508, Information Canada, Ottawa, Canada.
6. *Egeszegtudomány* 1980, 24, 173.
7. Gericke, P. et al *Test for Mutagenicity in Bacterial Strains in the Absence and Presence of a Liver Preparation* 1977, Unpublished Report No. 12/77, Hoechst.
8. Velasquez, A. et al *J. Toxicol. Environ. Health* 1990, 31(4), 313-315.
9. Mayor, D. et al *Test Report on the Mutagenicity of HOE02960 After Oral Administration to NMRI Mice, Micronucleus Test* 1980, Unpublished Report No. 81/80, Hoechst.
10. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
11. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
12. *1967 Directive on Classification, Packaging and Labelling of Dangerous Substances* 67/548/EEC; *7th Amendment EEC Directive* 91/32/EEC 1991, HMSO, London, UK.
13. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21

T206 tribromonitromethane



CBr_3NO_2

Mol. Wt. 297.73

CAS Registry No. 464-10-8

Synonyms bromopicrin; nitrobromoform; nitrotribromomethane

EINECS No. 207-348-4

RTECS No. PB 0100000

Uses Organic synthesis. Warfare agent.

Physical properties

M. Pt. 103°C **B. Pt.** 127°C at 118 mmHg **Specific gravity** 2.79 at 20°C with respect to water at 4°C

Solubility Water: <1 g l⁻¹ at 13°C. Organic solvents: acetic acid, acetone, benzene, diethyl ether, ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal mouse 15 mg kg⁻¹ (1).

Irritancy

Lachrymator and lung irritant (2).

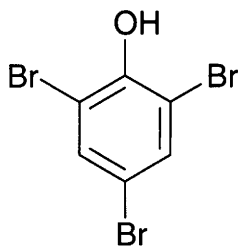
Other comments

Disinfectant by-product in drinking water (3).

References

1. *Khimikr-Format. Z.* 1976, 10(6), 53.
2. *Sax's Dangerous Properties of Industrial Materials* 8th ed., 1992, Van Nostrand Reinhold, New York, NY, USA.
3. Thibaud, H. et al *Water Res.* 1988, 22(3), 381-390

T207 2,4,6-tribromophenol



$\text{C}_6\text{H}_3\text{Br}_3\text{O}$

Mol. Wt. 330.80

CAS Registry No. 118-79-6

Synonyms Bromol

EINECS No. 204-278-6

RTECS No. SN 1225000

Uses Organic synthesis. Fire-proofing agent in polymers. Fungicide. Antiseptic.

Physical properties

M. Pt. 87-89°C **B. Pt.** 282-290°C at 746 mmHg **Specific gravity** 2.55 at 20°C with respect to water at 20°C
Partition coefficient $\log P_{ow}$ 4.020 (1) **Volatility** v.den. 11.4
Solubility Water: 71 mg l⁻¹ at 15°C. Organic solvents: chloroform, diethyl ether, ethanol, glycerols

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow 1.1 mg l⁻¹ flow-through bioassay (2).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 6.5 ppm Microtox test (3).

Environmental fate

Nitrification inhibition

IC₅₀ (25 day) *Nitrosomonas* sp. 7.7 mg l⁻¹ (2).

35% inhibition of nitrification by sewage sludge at 50 mg l⁻¹ (4).

Anaerobic effects

IC₅₀ (50 day) methanogenic bacterial culture 7.5 mg l⁻¹ (2).

Degradation studies

Undergoes microbial degradation in anoxic marine sediments via progressive debromination (5).

Degradation by *Pseudomonas* sp. 200 mg l⁻¹ at 30°C; 14% ring disruption in 120 hr by parent strain, 92% ring disruption by mutant in 42 hr (6).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 2000 mg kg⁻¹ (7).

Metabolism and toxicokinetics

Rapidly absorbed from the gastro-intestinal tract (8).

Irritancy

Irritating to the eyes, skin, mucous membranes and upper respiratory tract (9).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (10).

Other effects

Any other adverse effects

Toxic to primary rat hepatocytes at 125 mg l⁻¹ *in vitro* (11).

Decreased the respiration rate of rat liver mitochondria *in vitro* by inhibiting the NAD-dependent dehydrogenases (12).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (13).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (14).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (15).

Other comments

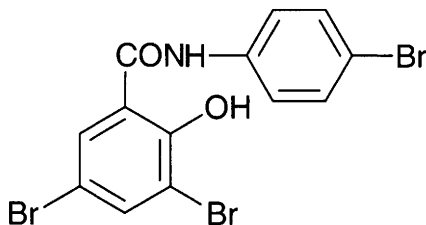
Detected in drinking water (11).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (16).

References

1. Schultz, T. W. et al *Bull. Environ. Contam. Toxicol.* 1989, **43**(2), 192-198.
2. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, **63**(3), 198-207.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. Wood, L. B. et al *Water Res.* 1981, **15**, 534-551.
5. Abrahamsson, K. et al *Mar. Pollut. Bull.* 1991, **22**(5), 227-233.
6. Worne, H. E. *Tijdschrift van Let BECEWA* Liege, Belgium.
7. Marhold, J. V. *Prehled Prumyslove Toxikologie: Organicke Latky* 1986, Prague, Czechoslovakia.
8. *Patty's Industrial Hygiene and Toxicology* 3rd ed., 1981, **2A**, 2615-2616, Wiley Interscience, New York, NY, USA.
9. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3394, Sigma-Aldrich, Milwaukee, WI, USA.
10. Zeiger, E. et al *Environ. Mutagen.* 1987, **9**(Suppl. 9), 1-109.
11. Murayama, J. et al *Eisei Kagaku* 1990, **36**(4), 267-276.
12. Ratnikova, L. A. et al *Mitokhondrii Mol. Mekh. Ferment. Reakts Meter. Uses Simp. Biokhim. Mitochondril* 1972, **6**, 77.
13. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
14. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
15. *1967 Directive on Classification, Packaging and Labelling of Dangerous Substances* 67/548/EEC; *6th Amendment EEC Directive* 79/831/EEC; *7th Amendment EEC Directive* 91/32/EEC 1991, HMSO, London, UK.
16. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T208 3,4',5-tribromosalicylanilide



$C_{13}H_8Br_3NO_2$

Mol. Wt. 449.92

CAS Registry No. 87-10-5

Synonyms 3,5-dibromo-N-(4-bromophenyl)-2-hydroxybenzamide; polybrominated salicylanilide; Temasept IV; TBS; tribromosalan; Tuasol

EINECS No. 201-723-6

RTECS No. VN 8925000

Physical properties

M. Pt. 227-228°C

Solubility Organic solvents: acetone, dimethylformamide

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 410 mg kg⁻¹ (1).

Sensitisation

Reported to have photoallergenic potential (2,3).

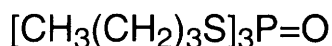
Legislation

Prohibited for use in cosmetics by US FDA (4).

References

1. *Ind. Med. Surg.* 1970, **39**, 56.
2. Lovel, H. H. et al *Toxicol. In Vitro* 1990, **4**(4-5), 318-320.
3. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
4. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA

T209 tribufos



$\text{C}_{12}\text{H}_{27}\text{OPS}_3$

Mol. Wt. 314.52

CAS Registry No. 78-48-8

Synonyms *S,S,S*-tributyl phosphorotrithioate; Butifos; butyl phosphorothioate; B-1776; Chemagro B-1776; DEF defoliant; DE-Green; Fos-Fall "A"; Ortho Phosphate Defoliant

EINECS No. 201-120-8

RTECS No. TG 5425000

Uses Insecticide. Herbicide. Cotton defoliant. Growth regulator.

Physical properties

M. Pt. $<-25^\circ\text{C}$ **B. Pt.** 150°C at 0.3 mmHg **Specific gravity** 1.0421 at 25°C with respect to water at 4°C

Partition coefficient $\log P_{\text{ow}}$ 3.2304 (1) **Volatility** v.p. 1.4×10^{-5} mmHg at 20°C

Solubility Water: 2.3 mg l^{-1} at 20°C . Organic solvents: acetone, benzene, chloroform, methanol, petroleum ether

Ecotoxicity

Fish toxicity

LC_{50} (96 hr) bluegill sunfish 1.0 mg l^{-1} (2).

LC_{50} (96 hr) rainbow trout <5 mg l^{-1} (2).

Invertebrate toxicity

Mysidopsis bahia continuous exposure to $0.25 \mu\text{g}^{-1}$ completely arrested reproduction (3).

LC_{50} (96 hr) *Gammarus lacustris* 100 $\mu\text{g} \text{l}^{-1}$ (4).

Relatively non-toxic to honeybees (1).

Bioaccumulation

Calculated bioconcentration factor of 12,600 indicates that environmental accumulation will occur (5).

Bioconcentration factor in pinfish 350 in 96 hr (6).

Environmental fate

Degradation studies

$>95\%$ loss in 8 wk due to biological process in river water (7).

Abiotic removal

Slowly hydrolysed under alkaline conditions (1).

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated $t_{1/2}$ 5 hr (8).

Estimated volatilisation $t_{1/2}$ 221 days from model river water; >4500 yr from model pond water taking into consideration the effect of adsorption (5,9).

Adsorption and retention

Estimated K_{oc} 30,000 indicates that adsorption to soil and sediments would be significant (5).

Rate of adsorption by soil $40 \text{ g kg}^{-1} \text{ soil hr}^{-1}$ (10).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird $>100 \text{ mg kg}^{-1}$ (11).

LD₅₀ oral rat, mouse, guinea pig, rabbit $77\text{--}330 \text{ mg kg}^{-1}$ (1,2,12-14).

LD₅₀ intraperitoneal rat, mouse 210, 290 mg kg^{-1} , respectively (15).

LD₅₀ intratracheal guinea pig 490 mg kg^{-1} (12).

LD₅₀ dermal rat, rabbit $100\text{--}850 \text{ mg kg}^{-1}$ (1,16,17).

Sub-acute and sub-chronic data

Oral rat (84 day) 25 mg kg^{-1} diet caused no adverse effects (15).

Teratogenicity and reproductive effects

Oral ♀ rat, lowest toxic dose 220 mg kg^{-1} 8 wk prior to mating – reproductive effects (18).

Irritancy

Dermal rabbit 35% aqueous emulsion caused slight erythema in 5-6 hr. 2-10% aqueous emulsion instilled into rabbit eye caused irritating effects (12).

Genotoxicity

In vitro Chinese hamster V79 cells, sister chromatid exchanges negative (metabolic activation unspecified) (19).

Other effects

Any other adverse effects

Cholinesterase inhibitor (12).

Caused morphological changes to erythrocytes and nuclear membranes, and affected the permeability properties of rat liver mitochondrial membrane, disrupting the calcium transport system and other energy-dependent mitochondrial processes (20).

Legislation

Maximum admissible concentration in open water bodies in former USSR $0.3 \mu\text{g l}^{-1}$ (12).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (21).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (22).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (23).

ADI $0.001 \text{ ng kg}^{-1} \text{ body weight}$ (1).

Other comments

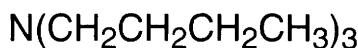
Use in former USSR discontinued.

References

1. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
2. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
3. McKenney, C. L. et al *Aquat. Toxicol.* 1991, **19**(2), 123-135.
4. Sanders, H. O. *Toxicity of Pesticides to the Crustacean Gammarus lacustris* 1969, Bureau of Sport Fisheries and Wildlife Technical Paper 25, Govt. Printing Office, Washington, DC, USA.
5. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
6. Environ. Res. Lab. *Report* 1981, 19-35, USEPA-600/4-81-041, Washington, DC, USA.

7. Eichelberger, J. W. et al *Environ. Sci. Technol.* 1971, **5**, 541-544.
8. Atkinson, R. *Environ. Toxicol. Chem.* 1988, **7**, 435-442.
9. EXAMS II Computer Simulation 1985, US EPA, Athens, GA, USA.
10. Aripov, E. A. et al *Uzb. Khim. Zh.* 1986, (2), 65-66 (Russ.) (*Chem. Abstr.* **106**, 14504v).
11. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
12. Kagan, Y. S. et al in Izmerov, W. F. *Scientific Reviews of Soviet Literature of Toxicity and Hazards of Chemicals* 1991, Moscow. (English Translation, Richardson, M. L. (Ed.) 1991, WHO, Geneva, Switzerland).
13. Marhold, J. V. *Prehled Prumyslove Toxikologie: Organické Latky* 1986, Prague, Czechoslovakia.
14. *Toxicol. Appl. Pharmacol.* 1969, **14**, 515.
15. Deichmann, W. B. *Toxicology of Drugs and Chemicals* 1969, 199, Academic Press, New York, NY, USA.
16. *World Rev. Pest Control* 1970, **9**, 119.
17. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
18. *Med. Z. Uzbek.* 1980, (2), 48.
19. Chem, H. H. et al *Mutat. Res.* 1982, **103**, 307.
20. Mirakhmedov, A. K. et al *Indian J. Exp. Biol.* 1989, **27**(3), 245-247.
21. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
22. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
23. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK

T210 tributylamine



$\text{C}_{12}\text{H}_{27}\text{N}$

Mol. Wt. 185.35

CAS Registry No. 102-82-9

Synonyms *N,N*-dibutyl-1-butanamine; tri-*n*-butylamine

EINECS No. 203-058-7

RTECS No. YA 0350000

Uses Catalyst. Corrosion inhibitor. Organic synthesis. Solvent.

Physical properties

M. Pt. -70°C B. Pt. 216°C Flash point 63°C Specific gravity 0.7782 at 20°C with respect to water at 20°C

Partition coefficient $\log P_{\text{ow}}$ 4.41 (1) Volatility v.p. 0.7 mmHg at 20°C ; v.den. 6.38

Solubility Water: sparingly soluble. Organic solvents: acetone, benzene, diethyl ether, ethanol

Occupational exposure

UN No. 2542 HAZCHEM Code 3X Conveyance classification corrosive substance

Ecotoxicity

Fish toxicity

LC_{50} (24 hr) creek chub, gudgeon $\sim 30 \text{ mg l}^{-1}$ (2-4).

Bioaccumulation

The calculated bioconcentration factor of 80 indicates that environmental accumulation would not be significant (5).

Environmental fate

Nitrification inhibition

Not inhibitory to ammonia oxidation by *Nitrosomonas* sp. at 100 mg l⁻¹ (6).

Degradation studies

Biodegradation 5% of ThOD in 15 days using Japanese industrial standards BOD dilution method with activated sludge inoculum (7).

Metabolism by *Candida utilis* believed to involve oxidation by a tertiary amine monooxygenase, to yield the aldehyde (8).

Abiotic removal

Volatilisation from model river water estimated $t_{1/2}$ 4.7 hr (5).

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated $t_{1/2}$ 3.9 hr (9).

Adsorption and retention

Estimated K_{oc} 570 indicates moderate adsorption to soil and sediments (5).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird >100 mg kg⁻¹ (10).

LD₅₀ oral rat, rabbit, guinea pig, mouse 110-615 mg kg⁻¹ (11,12).

LC_{Lo} (4 hr) inhalation rat 75 ppm (12).

LD₅₀ dermal rabbit 250 mg kg⁻¹ (12).

LD_{Lo} subcutaneous rat 380 mg kg⁻¹ (13).

Irritancy

Rabbit eye (24 hr) rated 1 (minimal effects) on a scale of 1-10 (14).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (15).

Other effects

Other adverse effects (human)

Extremely destructive to tissues of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema (16).

Any other adverse effects

Caused central nervous system stimulation, skin irritation and sensitisation (17).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (17).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (18).

Other comments

Environmental fate reviewed (19).

Mammalian toxicity and metabolism reviewed (20).

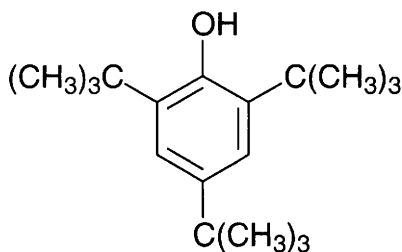
Reviews on human health effects, experimental toxicology, physico-chemical properties listed (21).

References

1. PCGEMS; *Graphical Exposure Modelling System* 1989, US EPA Office of Toxic Substances, Washington, DC, USA.
2. Gillette, L. A. et al *Sewage. Ind. Wastes* 1952, **24**(11), 1397-1401.

3. McKee, J. E. et al *Water Quality Criteria* 1963, Resources Agency of California, Static Water Quality Control Board.
4. Meinck, F. et al *Les Eau Residuaries Industrielle* 1970.
5. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
6. Hockenbury, M. R. et al *J. Water Pollut. Control Fed.* 1977, **49**(5), 768-777.
7. Yoshimura, K. et al *J. Am. Oil Chem. Soc.* 1980, **57**, 238-241.
8. Green, J. et al *J. Gen. Microbiol.* 1984, **130**, 2577-2588.
9. Atkinson, R. A. *Int. J. Chem. Kinet.* 1987, **19**, 799-828.
10. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
11. *Gig. Sanit.* 1977, **42**(12), 36.
12. *Toxicol. Appl. Pharmacol.* 1974, **28**, 313.
13. *J. Pharmacol. Exp. Therap.* 1923, **20**, 435.
14. Grant, W. M. *Toxicology of the Eye* 3rd ed., 1985, 1061, Charles C. Thomas, Springfield, IL, USA.
15. Zeiger, E. et al *Environ. Mutagen.* 1987, **9**(Suppl. 9), 1-109.
16. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3395, Sigma-Aldrich, Milwaukee, WI, USA.
17. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
18. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
19. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1991, **2**, 445-449, Lewis, Chelsea, MI, USA.
20. Buhler, D. R. et al (Eds.) *Ethel Browning's Toxicity and Metabolism of Industrial Solvents* 2nd ed., 1990, Elsevier, NY, USA.
21. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T211 2,4,6-tri-*tert*-butylphenol



C₁₈H₃₀O

Mol. Wt. 262.44

CAS Registry No. 732-26-3

Synonyms 2,4,6-tris(1,1-dimethylethyl)phenol; Alkofen B

EINECS No. 211-989-5

RTECS No. SN 3570000

Physical properties

M. Pt. 129-132°C **B. Pt.** 277°C **Partition coefficient** log P_{ow} 7.42 (1)

Occupational exposure

UN No. 2430

Ecotoxicity

Bioaccumulation

Confirmed to be bioaccumulated at a high level (2).

Nominal exposure concentration of 20 µg l⁻¹, measured exposure concentration of 13.9 µg l⁻¹; exposure period 4 wk, gave a normalised bioconcentration factor in common carp of 2524 (3).

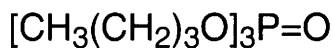
Legislation

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (4).

References

1. Schultz, T. W. et al *Bull. Environ. Contam. Toxicol.* 1989, **43**, 192-198.
2. *The list of existing chemical substances tested on biodegradability by microorganisms or accumulation in fish body* 1987, Chemicals Inspection and Testing Institute, Japan.
3. Tadokora, H. et al *QSAR Environ. Toxicol. II* 1987, 363-373.
4. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK

T212 tributyl phosphate



C₁₂H₂₇O₄P

Mol. Wt. 266.32

CAS Registry No. 126-73-8

Synonyms celluphos 4; TBP; tri-*n*-butyl phosphate

EINECS No. 204-800-2

RTECS No. TC 7700000

Uses Extracting metal complexes. In preparation of blood coagulation factors. Plasticiser.

Occurrence Detected in surface waters (1).

Physical properties

M. Pt. -79°C B. Pt. 180-183°C at 22 mmHg Flash point 193°C (open cup) Specific gravity 0.982 at 20°C

Volatility v.p. 17 mmHg at 177°C; v.den. 9.20

Solubility Water: 6 g l⁻¹. Organic solvents: benzene, carbon disulfide, diethyl ether, ethanol

Occupational exposure

FR-VME 0.2 ppm (2.5 mg m⁻³)

UK-LTEL 5 mg m⁻³

UK-STEL 5 mg m⁻³

US-TWA 0.2 ppm (2.2 mg m⁻³)

Supply classification harmful

Risk phrases Harmful if swallowed (R22)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with the eyes (S2, S25)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) silver carp, rainbow trout 5.0-9.0 mg l⁻¹ (2,3).

Invertebrate toxicity

Toxicity threshold cell multiplication inhibition test *Pseudomonas putida* >100 mg l⁻¹ *Scenedesmus quadricauda* 3.2 mg l⁻¹, *Entosiphon sulcatum* 14 mg l⁻¹ (4).

Environmental fate

Nitrification inhibition

Not inhibitory to nitrifying bacteria at 100 mg l⁻¹ (5).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 1200, 3000 mg kg⁻¹, respectively (6,7).

LC_{Lo} (5 hr) inhalation cat 24,000 mg m⁻³ (8).

LC₅₀ inhalation mouse 1300 mg m⁻³ (exposure unspecified) (7).

LD₅₀ intraperitoneal mouse, rat 160, 250 mg kg⁻¹, respectively (7).

LD_{Lo} intravenous rat 100 mg kg⁻¹ (9).

Intravenous rat, 80 mg kg⁻¹ caused light anaesthesia in 1 hr and 100 mg kg⁻¹ caused anaesthesia in 8-10 min, followed by respiratory failure (10).

Intraperitoneal rat, 16-270 mg kg⁻¹ doubled the activity of β -glucuronidase in plasma and inhibited plasma cholinesterase (10).

Carcinogenicity and chronic effects

♂ Sprague-Dawley rats (10 wk) 0-3000 ppm in diet. Tumours of the bladder urothelium were observed in rats receiving 700 and 3000 ppm (11).

Teratogenicity and reproductive effects

Oral ♂ rat, lowest toxic dose 12,600 mg kg⁻¹ day⁻¹ for 63 days – reproductive effects (12).

Oral rat, lowest toxic dose 7500 mg kg⁻¹ day⁻¹ on days 6-15 of gestation - foetotoxicity (13).

Dietary no-observed-adverse-effect level for reproductive toxicity in rats at least 3000 ppm and for postnatal toxicity ~200 ppm (14).

Metabolism and toxicokinetics

Absorbed through the skin of pigs (15).

Irritancy

Vapour or mist is irritating to the mucous membranes and upper respiratory tract (16).

Dermal rabbit (24 hr) 10 mg caused irritation (17).

500 mg instilled into rabbit eye caused severe irritation (exposure unspecified) (18).

Genotoxicity

Salmonella typhimurium TA1535, TA1538 with and without metabolic activation positive (19).

Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538 with and without metabolic activation negative (20).

Drosophila melanogaster sex-linked recessive lethal assay negative (10).

Other comments

Environmental fate and toxicology reviewed (21).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (22).

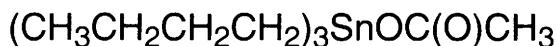
Autoignition temperature 410°C.

References

1. Pancorbo, O. C. et al *Arch. Environ. Contam. Toxicol.* 1987, **16**(5), 531-537.
2. Zhou, F. et al *Nanjing Daxue Xuebao, Ziran Kexue* 1989, **25**(3), 98-104 (Ch.) (*Chem. Abstr.* **112**, 153212b).
3. Verschuere, K. *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, 1119, Van Nostrand Reinhold, New York, NY, USA.
4. Bringmann, G. et al *Water Res.* 1980, **14**, 231-241.
5. Arenshtein, A. M. et al *Biokhim. Och. Stokhn.* 1962, 128-177 (*Chem. Abstr.* **61**, 15067h).
6. Smyth, H. F. et al *J. Ind. Hyg. Toxicol.* 1944, **26**, 269.
7. *Gig. Tr. Prof. Zabol.* 1971, **15**(8), 30.

8. Eller, H. *Beitrag zur Toxikologie Technischer Weichmachungsmittel* 1937, Univ. Wuerzburg, Germany.
9. *Nature* 1957, **179**, 154.
10. *Documentation of Threshold Limit Values* 4th ed., 1980, American Conference of Governmental Industrial Hygienists, Cincinnati, OH, USA.
11. Arnold, L. L. et al *Fundam. Appl. Toxicol.* 1997, **40**(2), 247-255.
12. *Toxicol. Lett.* 1982, **13**, 29.
13. *Report 8EHQ-0491-1007S*, US EPA Office of Pesticides and Toxic Substances.
14. Tyl, R. W. et al *Fundam. Appl. Toxicol.* 1997, **40**(1), 90-100.
15. LaDu, B. N. et al *Fundamentals of Drug Metabolism and Disposition* 1971, 40, Williams & Wilkins, Baltimore, USA.
16. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, 2, 3398, Sigma-Aldrich, Milwaukee, WI, USA.
17. *J. Ind. Hyg. Toxicol.* 1944, **26**, 269.
18. *Am. J. Ophthalm.* 1946, **29**, 1363.
19. Gafieva, Z. A. et al *Gig. Sanit.* 1986, (9), 81 (Russ.) (*Chem. Abstr.* **106**, 1660j).
20. Microbiological Associates *Activity of Tri-n-butyl Phosphate in the Salmonella/Microsomal Assay for Bacterial Mutagenicity* 1977, EPA Doc. No. 86860000112.
21. Williams, R. T. et al *Report* 1987, CRDEC-CR-8710. in *Gov. Rep. Announce. Index (US)* 1988, **88**(2), Abstr. No. 804,491.
22. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T213 tributyltin acetate



$\text{C}_{14}\text{H}_{30}\text{O}_2\text{Sn}$

Mol. Wt. 349.10

CAS Registry No. 56-36-0

Synonyms (acetyloxy)tributylstannane

EINECS No. 200-269-6

RTECS No. WH 6735000

Uses Antifouling agent. Catalyst.

Physical properties

M. Pt. 86-87°C

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Sn) (total dust)

SE-LEVL 0.1 mg m⁻³ (as Sn)

SE-STEL 0.2 mg m⁻³ (as Sn)

UK-LTEL 0.1 mg m⁻³ (as Sn)

UK-STEL 0.2 mg m⁻³ (as Sn)

US-TWA 0.1 mg m⁻³ (as Sn)

US-STEL 0.2 mg m⁻³ (as Sn)

UN No. 2788 (liquid); 3146 (solid) HAZCHEM Code 2X (solid) Conveyance classification toxic substance
Supply classification toxic

Risk phrases Harmful in contact with skin – Toxic if swallowed – Irritating to eyes and skin – Toxic: danger of serious damage to health by prolonged exposure through inhalation and if swallowed (R21, R25, R36/38, R48/23/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – This material and its container must be disposed of in a safe way – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S35, S36/37/39, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) red killifish 80 µg l⁻¹ (1).

Invertebrate toxicity

EC₅₀ (growth inhibition) *Skeletonema costatum*, *Thalassiosira pseudonana* 0.36-0.41 µg l⁻¹ (2).

Environmental fate

Degradation studies

Organotins can be degraded by light, but light may also stimulate photosynthetic organisms which carry out degradation (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 46, 99 mg kg⁻¹, respectively (4,5).

LD₅₀ intravenous mouse 180 mg kg⁻¹ (6).

LD_{Lo} intraperitoneal rat 10 mg kg⁻¹ (7).

Sub-acute and sub-chronic data

Oral rat 4, 8 or 16 mg kg⁻¹ 3 × wk⁻¹ for 5 wk caused histopathological lesions in the lungs, liver, intestine and kidneys (8).

Teratogenicity and reproductive effects

Oral rat, lowest toxic dose 175 mg kg⁻¹ day⁻¹ on days 7-17 of gestation (foetotoxicity, and craniofacial and musculoskeletal teratogenic effects) (9).

Other effects

Any other adverse effects

In experimental animals tributyltin compounds cause damage to the liver, haematological and endocrine systems and are irritating to the skin and eyes. Inhalation of aerosols leads to respiratory irritation (10).

Adverse effects to the immune system in rats have been reported. The no-observed-effect level for tributyltin compounds using the *Trichinella spiralis* host-resistance model in rats was 0.5-5.0 mg kg⁻¹ diet (10).

Legislation

Included in Schedules 5 and 6 (Release into Water and Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (11).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (12).

Included in Control of Pollution (Anti-fouling Paints and Treatments) Regulations 1987 (13).

Other comments

Exposure of workers to tributyltin compounds occurs mainly in the manufacture, application and removal of tributyltin paints and wood preservatives. Exposure of the general public may arise from the contamination of food, particularly fish and shellfish, and from domestic applications of wood preservatives (10).

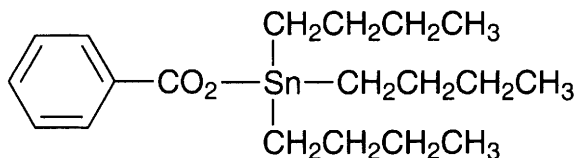
Toxicity of tributyltin compounds reviewed (10,14-16).

References

1. Nagess, H. et al *Appl. Organomet. Chem.* 1991, 5, 91-97.
2. Walsh, G. E. et al *Environ. Toxicol. Chem.* 1987, 6(10), 767-770.
3. Craig, P. J. (Ed.) *The Biological Alkylation of Heavy Elements* 1987, The Royal Society of Chemistry, London, UK.
4. *Arch. Toxikol.* 1968, 23, 283.

5. *J. Pharm. Sci.* 1967, **56**, 240.
6. Report NX 01672, US Army Armament Research and Development Command, Chemical Systems Laboratory, Aberdeen Proving Ground, MD 21010, USA.
7. *Br. J. Pharmacol. Chemotherap.* 1955, **10**, 16.
8. Attahuri, U. S. et al *Vet. Human Toxicol.* 1991, **33**(5), 499-502.
9. *Toxicol. Lett.* 1991, **55**, 109.
10. *IPCS Environmental Health Criteria 116: Tributyltin Compounds* 1990, WHO, Geneva, Switzerland.
11. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
12. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
13. *S. I.* 1987, No. 783 *Control of Pollution (Anti-fouling Paints and Treatments) Regulations* 1987, HMSO, London, UK.
14. Thayer, J. S. et al *Adv. Organomet. Chem.* 1982, **20**, 313.
15. Thompson, J. A. J. et al *Organotin Compounds in the Aquatic Environment* 1985, National Res. Council Canada, NRCC2294, Canada.
16. Byrne, C. D. *Selection of Substances Requiring Priority Action* in Richardson, M. L. (Ed.) *Risk Assessment of Chemicals in the Environment* 1988, 414-436, The Royal Society of Chemistry, London, UK

T214 tributyltin benzoate



$C_{19}H_{32}O_2Sn$

Mol. Wt. 411.17

CAS Registry No. 4342-36-3

Synonyms (benzoyloxy)tributylstannane

EINECS No. 224-399-8

RTECS No. WH 6710000

Uses Fungicide used in skin treatment preparations.

Physical properties

M. Pt. 21-22°C B. Pt. 166-168°C at 1 mmHg Flash point >110°C Specific gravity 1.1973 at 20°C

Occupational exposure

DE-MAK 0.0021 ppm (0.05 mg m⁻³) (as TBTO)

SE-LEVL 0.1 mg m⁻³ (as Sn)

SE-STEEL 0.2 mg m⁻³ (as Sn)

UK-LTEL 0.1 mg m⁻³ (as Sn)

UK-STEEL 0.2 mg m⁻³ (as Sn)

US-TWA 0.1 mg m⁻³ (as Sn)

US-STEEL 0.2 mg m⁻³ (as Sn)

UN No. 2788 (liquid); 3146 (solid) HAZCHEM Code 2X (solid) Conveyance classification toxic substance
Supply classification toxic

Risk phrases Harmful in contact with skin – Toxic if swallowed – Irritating to eyes and skin – Toxic: danger of serious damage to health by prolonged exposure through inhalation and if swallowed (R21, R25, R36/38, R48/23/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – This material and its container must be disposed of in a safe way – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S35, S36/37/39, S45)

Environmental fate

Degradation studies

Organotins can be degraded by light, but light may also stimulate photosynthetic organisms which carry out degradation (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 110, 130 mg kg⁻¹, respectively (2,3).

LD₅₀ dermal rat 500 mg kg⁻¹ (2).

LD₅₀ intravenous mouse 180 mg kg⁻¹ (4).

Other effects

Any other adverse effects

In experimental animals, tributyltin compounds cause damage to the liver, haematological and endocrine systems and are irritating to the skin and eyes. Inhalation of aerosols leads to respiratory irritation (5).

Adverse effects to the immune system in rats have been reported. The no-observed-effect level for tributyltin compounds using the *Trichinella spiralis* host-resistance model in rats was 0.5-5.0 mg kg⁻¹ diet (5).

Legislation

Included in Schedule 5 (Release into Water: Prescribed Substances) Statutory Instrument No. 472, 1991 (6).

Other comments

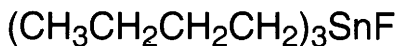
Toxicity of tributyltin compounds reviewed (5,7-9).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (10).

References

1. Craig, P. J. (Ed.) *The Biological Alkylation of Heavy Elements* 1987, The Royal Society of Chemistry, London, UK.
2. *Arzneim.-Forsch.* 1969, **19**, 934.
3. *Archiv. Toxikol* 1968, **23**, 283.
4. *Report*, US Army Armament Research and Development Command, Chemical Systems Laboratory, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD21010, USA.
5. *IPCS Environmental Health Criteria No. 116: Tributyltin Compounds* 1990, WHO, Geneva, Switzerland.
6. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
7. Thompson, J. A. J. et al *Organotin Compounds in the Aquatic Environment* 1985, National Research Council Canada, Assoc. Comm. Sci. Criteria Environ. Qual. Publ. No. NRCC2294.
8. Byrne, C. D. *Selection of Substances Requiring Priority Action* in Richardson, M. L. (Ed.) *Risk Assessment of Chemicals in the Environment* 1988, 414-436, The Royal Society of Chemistry, London, UK.
9. Thayer, J. S. et al *Adv. Organomet. Chem.* 1982, **20**, 313.
10. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T215 tributyltin fluoride



$\text{C}_{12}\text{H}_{27}\text{FSn}$

Mol. Wt. 309.05

CAS Registry No. 1983-10-4

Synonyms fluorotributylstannane; tributylfluorostannane

EINECS No. 217-847-9

RTECS No. WH 8275000

Uses Manufacture of tributyltin fluoride polymer. Antifouling agent. Catalyst.

Occupational exposure

DE-MAK 0.0021 ppm (0.05 mg m⁻³) (as TBTO)

SE-LEVL 0.1 mg m⁻³ (as Sn)

SE-STEL 0.2 mg m⁻³ (as Sn)

UK-LTEL 0.1 mg m⁻³ (as Sn)

UK-STEL 0.2 mg m⁻³ (as Sn)

US-TWA 0.1 mg m⁻³ (as Sn)

US-STEL 0.2 mg m⁻³ (as Sn)

UN No. 2788 (liquid); 3146 (solid) HAZCHEM Code 2X (solid) Conveyance classification toxic substance

Supply classification toxic

Risk phrases Harmful in contact with skin – Toxic if swallowed – Irritating to eyes and skin – Toxic: danger of serious damage to health by prolonged exposure through inhalation and if swallowed (R21, R25, R36/38, R48/23/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – This material and its container must be disposed of in a safe way – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S35, S36/37/39, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) red killifish 62 µg l⁻¹ (1).

Invertebrate toxicity

Toxicity threshold (62 min) *Bacillus subtilis* ~30 µg l⁻¹ (2).

EC₅₀ (growth inhibition) *Skeletonema costatum* 0.36-0.39 µg l⁻¹ (3).

Environmental fate

Degradation studies

Organotins can be degraded by light, but light may also stimulate photosynthetic organisms which carry out degradation (4).

Mammalian & avian toxicity

Acute data

LD_{Lo} oral mouse, rabbit 50, 320 mg kg⁻¹, respectively (5,6).

Metabolism and toxicokinetics

Following oral administration of 6.5 mg kg⁻¹ to rats, tributyltin fluoride accumulated rapidly in the liver for 1 day, then decreased with t_{1/2} 4.1 days (7).

Genotoxicity

In vitro Chinese hamster ovary cells chromosomal aberrations with and without metabolic activation negative (8).

Other effects

Any other adverse effects

In experimental animals tributyltin compounds cause damage to the liver, haematological and endocrine systems and are irritating to the skin and eyes. Inhalation of aerosols leads to respiratory irritation (9).

Adverse effects to the immune system in rats have been reported. The no-observed-effect level for tributyltin compounds using the *Trichinella spiralis* host-resistance model in rats was 0.5-5.0 mg kg⁻¹ diet (9).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Fluorides: maximum admissible concentration 1500 µg l⁻¹ for water temperatures of 8-12°C, 700 µg l⁻¹ for water temperatures fo 25-30°C.

Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (10).

Included in Schedules 5 and 6 (Release into Water and Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (11).

Included in Control of Pollution (Anti-Fouling Paints and Treatments) Regulations 1987 (12).

Other comments

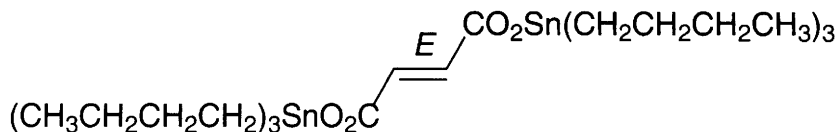
Toxicity of tributyltin compounds reviewed (9,13-15).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (16).

References

1. Nagese, H. et al *Appl. Organomet. Chem.* 1991, 5, 91-97.
2. Felkner, I. C. et al *Chem. Speciat. Bioavail.* 1989, 1(3), 79-92.
3. Walsh, G. E. et al *Environ. Toxicol. Chem.* 1987, 6(10) 876-770.
4. Craig, P. J. (Ed.) *The Biological Alkylation of Heavy Elements* 1987, The Royal Society of Chemistry, London, UK.
5. *Arch. Environ. Contam. Toxicol.* 1985, 14, 111.
6. *Sangyo Igaku* 1973, 15, 3.
7. Hada, N. et al *Nichidai Igaku Zasshi* 1986, 45(11), 1005-1013 (Japan.) (*Chem. Abstr.* 106, 97672p).
8. Sasaki, Y. F. et al *Mutat. Res.* 1993, 300, 5-14.
9. *IPCS Environmental Health Criteria No. 116: Tributyltin Compounds* 1990, WHO, Geneva, Switzerland.
10. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
11. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
12. *S. I. 1987, No. 783 Control of Pollution (Anti-Fouling Paints and Treatments) Regulations* 1987, HMSO, London, UK.
13. Thayer, J. S. et al *Adv. Organomet. Chem.* 1982, 20, 313.
14. Thompson, J. A. J. et al *Organotin Compounds in the Aquatic Environment* 1985, National Research Council Canada, Assoc. Comm. Sci. Criteria Environ. Qual. Publ. No. NRCC2294.
15. Byrne, C. D. *Selection of Substances Requiring Priority Action* in Richardson, M. L. (Ed.) *Risk Assessment of Chemicals in the Environment* 1988, 414-436, The Royal Society of Chemistry, London, UK.
16. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T216 tributyltin fumarate



$\text{C}_{28}\text{H}_{56}\text{O}_4\text{Sn}_2$

Mol. Wt. 694.17

CAS Registry No. 56323-17-2

Synonyms (fumaroyldioxy)bis[tributyltin]; 5,5,12,12-tetrabutyl-7,10-dioxo-6,11-dioxo-5,12-distanna-hexadec-8-ene; bis(tributyltin)fumarate; bis(tributylstannane)fumarate

Uses Antifouling agent. Manufacture of polymers.

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Sn) (total dust)

SE-LEVL 0.1 mg m⁻³ (as Sn)

SE-STEL 0.2 mg m⁻³ (as Sn)

UK-LTEL 0.1 mg m⁻³ (as Sn)

UK-STEL 0.2 mg m⁻³ (as Sn)

US-TWA 0.1 mg m⁻³ (as Sn)

US-STEL 0.2 mg m⁻³ (as Sn)

UN No. 2788 (liquid); 3146 (solid) **HAZCHEM Code** 2X (solid) **Conveyance classification** toxic substance
Supply classification toxic

Risk phrases Harmful in contact with skin – Toxic if swallowed – Irritating to eyes and skin – Toxic: danger of serious damage to health by prolonged exposure through inhalation and if swallowed (R21, R25, R36/38, R48/23/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – This material and its container must be disposed of in a safe way – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S35, S36/37/39, S45)

Environmental fate

Degradation studies

Organotins can be degraded by light, but light may also stimulate photosynthetic organisms which carry out degradation (1).

Other effects

Any other adverse effects

In experimental animals, tributyltin compounds cause damage to the liver, haematological and endocrine systems and are irritating to the skin and eyes. Inhalation of aerosols leads to respiratory irritation (2).

Adverse effects to the immune system in rats have been reported. The no-observed-effect level for tributyltin compounds using the *Trichinella spiralis* host-resistance model in rats was 0.5-5.0 mg kg⁻¹ diet (2).

Legislation

Included in Schedules 5 and 6 (Release into Water and Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (3).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (4).

Included in Control of Pollution (Anti-Fouling Paints and Treatments) Regulations 1987 (5).

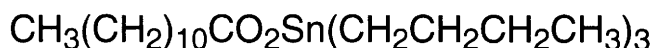
Other comments

Exposure of workers to tributyltin compounds occurs mainly in the manufacture, application and removal of tributyltin paints and wood preservatives. Exposure of the general public may arise from the contamination of food, particularly fish and shellfish, and from domestic applications of wood preservatives (2). Toxicity of tributyltin compounds reviewed (2,6-8).

References

1. Craig, P. J. (Ed.) *The Biological Alkylation of Heavy Elements* 1987, The Royal Society of Chemistry, London, UK.
2. *IPCS Environmental Health Criteria No. 116: Tributyltin Compounds* 1990, WHO, Geneva, Switzerland.
3. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
5. *S. I. 1987, No. 783 Control of Pollution (Anti-Fouling Paints and Treatments) Regulations* 1987, HMSO, London, UK.
6. Thayer, J. S. et al *Adv. Organomet. Chem.* 1982, **20**, 313.
7. Thompson, J. A. J. et al *Organotin Compounds in the Aquatic Environment* 1985, National Research Council Canada, Assoc. Comm. Sci. Criteria Environ. Qual. Publ. No. NRCC2294.
8. Byrne, C. D. *Selection of Substances Requiring Priority Action* in Richardson, M. L. (Ed.) *Risk Assessment of Chemicals in the Environment* 1988, 414-436, The Royal Society of Chemistry, London, UK

T217 tributyltin laurate



$\text{C}_{24}\text{H}_{50}\text{O}_2\text{Sn}$

Mol. Wt. 489.37

CAS Registry No. 3090-36-6

Synonyms (lauroyloxy)tributylstannane; Rustol-HED; tributyl[(1-oxododecyl)oxy]stannane; tributyltin dodecanoate

EINECS No. 221-434-9

RTECS No. WH 8584000

Uses Polymerisation catalyst. Manufacture of deodorants. Fungicide. Antifouling agent.

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Sn) (total dust)

SE-LEVL 0.1 mg m⁻³ (as Sn)

SE-STEL 0.2 mg m⁻³ (as Sn)

UK-LTEL 0.1 mg m⁻³ (as Sn)

UK-STEL 0.2 mg m⁻³ (as Sn)

US-TWA 0.1 mg m⁻³ (as Sn)

US-STEL 0.2 mg m⁻³ (as Sn)

UN No. 2788 (liquid); 3146 (solid) HAZCHEM Code 2X (solid) Conveyance classification toxic substance
Supply classification toxic

Risk phrases Harmful in contact with skin – Toxic if swallowed – Irritating to eyes and skin – Toxic: danger of serious damage to health by prolonged exposure through inhalation and if swallowed (R21, R25, R36/38, R48/23/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – This material and its container must be disposed of in a safe way – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S35, S36/37/39, S45)

Environmental fate

Degradation studies

Organotins can be degraded by light, but light may also stimulate photosynthetic organisms which carry out degradation (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 180 mg kg⁻¹ (2).

LD₅₀ intravenous mouse 20 mg kg⁻¹ (3).

Other effects

Other adverse effects (human)

A group of 35 exposed fabric workers was examined. Complaints, especially for upper respiratory tract diseases, were investigated. No indication of risks of an occupational disease was identified (4).

Any other adverse effects

In experimental animals tributyltin compounds cause damage to the liver, haematological and endocrine systems and are irritating to the skin and eyes. Inhalation of aerosols leads to respiratory irritation (5).

Adverse effects to the immune system in rats have been reported. The no-observed-effect level for tributyltin compounds using the *Trichinella spiralis* host-resistance model in rats was 0.5-5.0 mg kg⁻¹ diet (5).

Legislation

Included in Schedules 5 and 6 (Release into Water and Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (6).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (7).

Included in Control of Pollution (Anti-Fouling Paints and Treatments) Regulations 1987 (8).

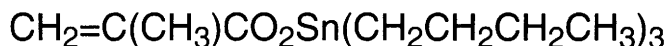
Other comments

Toxicity of tributyltin compounds reviewed (5,9-11).

References

1. Craig, P. J. (Ed.) *The Biological Alkylation of Heavy Elements* 1987, The Royal Society of Chemistry, London, UK.
2. *Arch. Toxikol.* 1968, **23**, 283.
3. *Report NX 02760*, US Army Armament Research and Development Command, Chemical Systems Laboratory, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD, USA.
4. Hassmonova, V. et al *Proc. Lek.* 1990, **42**(8), 341-344 (Czech.) (*Chem. Abstr.* **115**, 98351f).
5. *IPCS Environmental Health Criteria No. 116: Tributyltin Compounds* 1990, WHO, Geneva, Switzerland.
6. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
7. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
8. *S. I.* 1987, No. 783 *Control of Pollution (Anti-Fouling Paints and Treatments) Regulations* 1987, HMSO, London, UK.
9. Thayer, J. S. et al *Adv. Organomet. Chem.* 1982, **20**, 313.
10. Thompson, J. A. J. et al *Organotin Compounds in the Aquatic Environment* 1985, National Research Council Canada, Assoc. Comm. Sci. Criteria Environ. Qual. Publ. No. NRCC2294.
11. Byrne, C. D. *Selection of Substances Requiring Priority Action* in Richardson, M. L. (Ed.) *Risk Assessment of Chemicals in the Environment* 1988, 414-436, The Royal Society of Chemistry, London, UK

T218 tributyltin methacrylate



$\text{C}_{16}\text{H}_{32}\text{O}_2\text{Sn}$

Mol. Wt. 375.14

CAS Registry No. 2155-70-6

Synonyms tributyl(methacryloxy)stannane; tributyl[(2-methyl-1-oxo-2-propenyl)oxy]stannane; tributylstannyl methacrylate

EINECS No. 218-452-4

RTECS No. WH 8692000

Uses Manufacture of polymers. Antifouling agent.

Physical properties

M. Pt. 20-22°C B. Pt. 170-170.5°C

Occupational exposure

DE-MAK 0.0021 ppm (0.05 mg m⁻³) (as TBTO)

SE-LEVL 0.1 mg m⁻³ (as Sn)

SE-STEEL 0.2 mg m⁻³ (as Sn)

UK-LTEL 0.1 mg m⁻³ (as Sn)

UK-STEEL 0.2 mg m⁻³ (as Sn)

US-TWA 0.1 mg m⁻³ (as Sn)

US-STEEL 0.2 mg m⁻³ (as Sn)

UN No. 2788 (liquid); 3146 (solid) **HAZCHEM Code** 2X (solid) **Conveyance classification** toxic substance
Supply classification toxic

Risk phrases Harmful in contact with skin – Toxic if swallowed – Irritating to eyes and skin – Toxic: danger of serious damage to health by prolonged exposure through inhalation and if swallowed (R21, R25, R36/38, R48/23/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – This material and its container must be disposed of in a safe way – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S35, S36/37/39, S45)

Ecotoxicity

Invertebrate toxicity

IC₅₀ (48 hr) *Artemia salina* 1.24 mg l⁻¹ (1).

Environmental fate

Degradation studies

Organotins can be degraded by light, but light may also stimulate photosynthetic organisms which carry out degradation (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse, guinea pig 150-160 mg kg⁻¹ (3,4).

LD₅₀ intravenous mouse 18 mg kg⁻¹ (5).

Other effects

Any other adverse effects

In experimental animals, tributyltin compounds cause damage to the liver, haematological and endocrine systems, and are irritating to the skin and eyes. Inhalation of aerosols leads to respiratory irritation (6).

Adverse effects to the immune system in rats have been reported. The no-observed-effect level for tributyltin compounds using the *Trichinella spiralis* host-resistance model in rats 0.5-5.0 mg kg⁻¹ diet (6).

Legislation

Included in Schedules 5 and 6 (Release into Water and Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (7).

Included in Control of Pollution (Anti-Fouling Paints and Treatments) Regulations 1987 (8).

Other comments

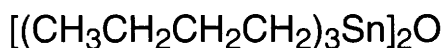
Toxicity of tributyltin compounds reviewed (6,9-11).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (12).

References

1. Dharia, J. R. et al *Toxicol. Environ. Chem.* 1989, **24**(3), 149.
2. Craig, P. J. (Ed.) *The Biological Alkylation of Heavy Elements* 1987, The Royal Society of Chemistry, London, UK.
3. *Ukrain. Biokhim. Z.* 1978, **50**, 695.
4. *Gig. Sanit.* 1975, **40**(4), 42.
5. Report US Army Armament Research and Development Command, Chemical Systems Laboratory, Aberdeen Proving Ground, MD 21010, USA.
6. *IPCS Environmental Health Criteria No. 116: Tributyltin Compounds* 1990, WHO, Geneva, Switzerland.
7. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
8. S. I. 1987, No. 783 *Control of Pollution (Anti-Fouling Paints and Treatments) Regulations* 1987, HMSO, London, UK.
9. Thayer, J. S. et al *Adv. Organomet. Chem.* 1982, **20**, 313.
10. Thompson, J. A. J. et al *Organotin Compounds in the Aquatic Environment* 1985, National Research Council Canada, Assoc. Comm. Sci. Criteria Environ. Qual. Publ. No. NRCC2294.
11. Byrne, C. D. *Selection of Substances Requiring Priority Action* in Richardson, M. L. (Ed.) *Risk Assessment of Chemicals in the Environment* 1988, 414-436, The Royal Society of Chemistry, London, UK.
12. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T219 tributyltin oxide



$\text{C}_{24}\text{H}_{54}\text{OSn}_2$

Mol. Wt. 596.11

CAS Registry No. 56-35-9

Synonyms biomet TBTO; bis(tributyltin) oxide; bis(tributylstannyl) oxide; BTO; butinox; C-Sn-9; hexabutylidistannoxane; TBTO

EINECS No. 200-268-0

RTECS No. JN 8750000

Uses Antifouling agent. Polymerisation catalyst. Superseded fungicide and bactericide.

Physical properties

M. Pt. -45°C **B. Pt.** 180°C at 2 mmHg **Flash point** above 112°C **Specific gravity** 1.14

Partition coefficient $\log P_{\text{ow}}$ 2.2 (1) **Volatility** v.p. <1 mmHg at 20°C

Solubility Water: 100 mg l^{-1} . Organic solvents: diethyl ether, ethanol

Occupational exposure

DE-MAK 0.0021 ppm (0.05 mg m^{-3}) (as TBTO)

SE-LEVL 0.1 mg m^{-3} (as Sn)

SE-STEL 0.2 mg m^{-3} (as Sn)

UK-LTEL 0.1 mg m^{-3} (as Sn)

UK-STEL 0.2 mg m^{-3} (as Sn)

US-TWA 0.1 mg m^{-3} (as Sn)

US-STEL 0.2 mg m^{-3} (as Sn)

UN No. 2788 (liquid); 3146 (solid) HAZCHEM Code 2X (solid) Conveyance classification toxic substance
Supply classification toxic

Risk phrases Harmful in contact with skin – Toxic if swallowed – Irritating to eyes and skin – Toxic: danger of serious damage to health by prolonged exposure through inhalation and if swallowed (R21, R25, R36/38, R48/23/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – This material and its container must be disposed of in a safe way – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S35, S36/37/39, S45)

Ecotoxicity

Fish toxicity

Three-spined stickleback (7.5 month) 0, 0.1, 1.0, 2.5 or 10 $\mu\text{g l}^{-1}$ flow-through bioassay in seawater. The highest dose was fatal to 80% of the fish within 2 months (2).

LC₅₀ (24, 96 hr) salt water goby, rainbow trout, fathead minnow 3-31 $\mu\text{g l}^{-1}$ (3-5).

Salt water goby 0.21-2.1 $\mu\text{g l}^{-1}$ for 12 wk reduced the number of germ cells in the testes, but spermatogenesis was not significantly inhibited (3).

LC₅₀ (96 hr) bleak, cichlid 15 53 $\mu\text{g l}^{-1}$, respectively (4,6).

Tributyltin oxide has been shown not to cause effects that mimic the action of steroids in fish species medaka and guppy (7).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 1.1 $\mu\text{g l}^{-1}$ Microtox test (8).

EC₅₀ (growth inhibition) *Skeletonema costatum*, *Thalassiosira pseudonana* 0.33-1.1 $\mu\text{g l}^{-1}$ (9).

LC₅₀ (96 hr) post larval and juvenile shrimp (in seawater) 19.4 and 370 $\mu\text{g l}^{-1}$, respectively (10).

Bioaccumulation

Salt water goby exposed to 0.21-2.1 $\mu\text{g l}^{-1}$ for 12 wk bioaccumulation factor 2000-11,000 (3).

Bioaccumulation factor in goldfish muscle 2800 following exposure to 1 $\mu\text{g l}^{-1}$ for 12 days. Depuration $t_{1/2}$ 6 days (11).

Environmental fate

Degradation studies

Biodegradation $t_{1/2}$ 4 months in water/sediment mixture derived from Toronto Harbour (12).

Adsorption and retention

K_{oc} 90,800 for Toronto Harbour sediments (13).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird >30 mg kg⁻¹ (14).

LD₅₀ oral rabbit, mouse, rat 50, 55, 190 mg kg⁻¹, respectively (15-17).

LD₅₀ dermal rabbit 900 mg kg⁻¹ (18).

LD₅₀ intravenous mouse 6 mg kg⁻¹ (18).

LD₅₀ intraperitoneal rat, mouse 7, 13 mg kg⁻¹, respectively (19,20).

Sub-acute and sub-chronic data

Oral rat 0, 0.5, 2.5, 5.0 or 50 mg kg⁻¹ in diet for 28 days. No treatment-related effects were noted on clinical chemistry and haematological parameters and on immune function, as determined by plaque-forming cell assay and delayed-type hypersensitivity response. Thymic atrophy and impaired immune function, as determined by impaired clearance of *Listeria monocytogenes* were noted only in the high-dose group (21).

Teratogenicity and reproductive effects

Oral rat, lowest toxic dose 150 mg kg⁻¹ day⁻¹ on days 6-20 of gestation – foetotoxicity, foetal death, teratogenicity (central nervous system) (22).

Metabolism and toxicokinetics

Absorbed through the skin of mammals (23).

Irritancy

50 µg instilled into rabbit eye for 24 hr caused severe irritation (24).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535 with and without metabolic activation negative (25).

Drosophila melanogaster sex-linked recessive lethal assay negative (26).

In vitro Chinese hamster cells with and without metabolic activation sister chromatid exchanges negative (26).

In vivo mouse erythrocytes, induction of micronuclei positive (26).

Other effects

Other adverse effects (human)

Extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema (27).

Exposure of workers to tributyltin compounds occurs mainly in the manufacture, application and removal of tributyltin paints and wood preservatives. Exposure of the general public may arise from the contamination of food, particularly fish and shellfish, and from domestic applications of wood preservatives (28).

Any other adverse effects

Macrophage secretory function was enhanced in B6C3F1 mice exposed to a single low dose 0.3, 3.0, or 30 mg kg⁻¹ tributyltin-oxide (29).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (30).

Included in Control of Pollution (Anti-Fouling Paints and Treatments) Regulations 1987 (31).

WHO guidelines value for drinking water 2 µg l⁻¹ (32).

Other comments

Environmental impact reviewed (33).

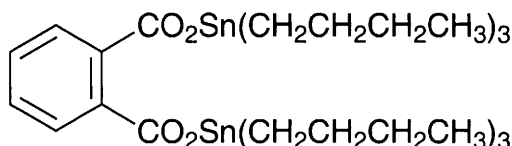
Physical properties, use, occurrence, metabolism and toxicity of tributyltin compounds reviewed (34,35).

References

1. Tsude, T. et al *Water Res.* 1988, **22**(5), 647-651.
2. Holm, G. et al *J. Fish Biol.* 1991, **38**(3), 373-386.
3. Shimizu, A. et al *Tokai-ku Suisan Kenkyasho Kerkyu Hokoku* 1987, (123), 45-59 (Japan.) (*Chem. Abstr.* **110**, 19601h).
4. Chliamovitch, Y.-P. et al *J. Fish Biol.* 1977, **10**, 575.
5. Geiger, D. L. et al (Eds.) *Acute Toxicities of Organic Chemicals to Fathead Minnows* 1990, **V**, 275, Univ. Wisconsin Superior, USA.
6. Linden, E. et al *Chemosphere* 1979, **11/12**, 843-851.
7. Wester, P. W. et al *Aquatic Toxicol.* 1990, **16**, 53-72.
8. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
9. Walsh, G. E. et al *Environ. Toxicol. Chem.* 1987, **6**(10), 767-770.
10. Lignot, J.-H. et al *Aquat. Toxicol.* 1998, **41**(4), 277-299.
11. Hada, N. *Nichidai Igaku Zasshi* 1986, **45**(11), 1005-1013 (Japan.) (*Chem. Abstr.* **106**, 97672p).
12. Maguire, R. J. *Preprint in ACS Natl. Meet.* 1984, **24**, 75-77.
13. Maguire, R. J. *J. Agric. Food Chem.* 1985, **33**, 947-953.
14. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
15. *Sangyo Igaku* 1973, **15**, 3.
16. *Gig. Sanit.* 1976, **41**(5), 10.

17. *The Pesticide Manual* 9th ed., 1991, British Crop Protection Council, Farnham, Surrey, UK.
18. *Eur. J. Toxicol. Environ. Hyg.* 1976, **9**, 31.
19. *Food Cosmet. Toxicol.* 1969, **7**, 47.
20. *Russ. Pharmacol. Toxicol.* 1979, **42**, 73.
21. Verdier, F. et al *J. Toxicol. Environ. Health* 1991, **32**(3), 307-317.
22. *Toxicol. Appl. Pharmacol.* 1989, **97**, 113.
23. Elsea, J. R. et al *AMA Arch. Ind. Health* 1958, **18**, 214.
24. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysvetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
25. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-58.
26. Davis, A. et al *Mutat. Res.* 1987, **188**(2), 65-95.
27. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **1**, 450, Sigma-Aldrich, Milwaukee, WI, USA.
28. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
29. Kergosien, D. H. et al *Arch. Environ. Contam. Toxicol.* 1998, **34**(3), 223-228.
30. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
31. S. I. 1987, No. 783 *Control of Pollution (Anti-Fouling Paints and Treatments) Regulations* 1987, HMSO, London, UK.
32. *Guidelines for Drinking Water Quality* 2nd ed., 1993, **1**, WHO, Geneva, Switzerland.
33. Bressa, G. D. A. *Dif. Ambientale* 1989, **13**(2), 26-29.
34. *IPCS Environmental Health Criteria* No. 116 *Tributyltin Compounds* 1990, WHO, Geneva, Switzerland.
35. *ECETOC Technical Report* No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T220 tributyltin phthalate



$C_{32}H_{58}O_4Sn_2$

Mol. Wt. 744.23

CAS Registry No. 4782-29-0

Synonyms [1,2-phenylenebis(carbonyloxy)]bis(tributylstannane); (phthaloyldioxy)bis(tributyltin); bis(tributyltin) phthalate

Uses Fungicide. Termiticide for rubbers and plastics. Antifouling agent.

Physical properties

M. Pt. 35-36°C

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Sn) (total dust)

SE-LEVL 0.1 mg m⁻³ (as Sn)

UK-LTEL 0.1 mg m⁻³ (as Sn)

US-TWA 0.1 mg m⁻³ (as Sn)

SE-STEEL 0.2 mg m⁻³ (as Sn)

UK-STEEL 0.2 mg m⁻³ (as Sn)

US-STEEL 0.2 mg m⁻³ (as Sn)

UN No. 2788 (liquid); 3146 (solid) **HAZCHEM Code** 2X (solid) **Conveyance classification** toxic substance

Supply classification toxic

Risk phrases Harmful in contact with skin – Toxic if swallowed – Irritating to eyes and skin – Toxic: danger of serious damage to health by prolonged exposure through inhalation and if swallowed (R21, R25, R36/38, R48/23/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – This material and its container must be disposed of in a safe way – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S35, S36/37/39, S45)

Environmental fate

Degradation studies

Organotins can be degraded by light, but light may also stimulate photosynthetic organisms which carry out degradation (1).

Mammalian & avian toxicity

Irritancy

Tributyltin compounds are irritants to the skin and eyes; inhalation of aerosols leads to respiratory irritation (2).

Other effects

Any other adverse effects

In experimental animals tributyltin compounds cause damage to the liver, haematological and endocrine systems, and are irritating to the skin and eyes. Inhalation of aerosols leads to respiratory irritation (2).

Adverse effects to the immune system in rats have been reported. The no-observed-effect level for tributyltin compounds using the *Trichinella spiralis* host-resistance model in rats 0.5-5.0 mg kg⁻¹ diet (2).

Legislation

Included in Schedules 5 and 6 (Release into Water and Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (3).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (4).

Included in Control of Pollution (Anti-Fouling Paints and Treatments) Regulations 1987 (5).

Other comments

Exposure of workers to tributyltin compounds occurs mainly in the manufacture, application and removal of tributyltin paints and wood preservatives. Exposure of the general public may arise from the contamination of food, particularly fish and shellfish, and from domestic applications of wood preservatives (2).

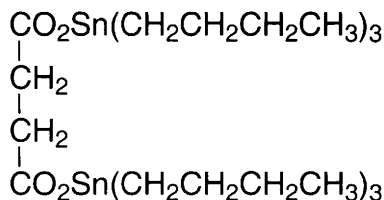
A deuteromycete, *Graphium* sp. M-19, degraded beech sapwood blocks treated with <0.1% tributyltin phthalate (6).

Toxicity of tributyltin compounds reviewed (2,7-9).

References

1. Craig, P. J. et al *The Biological Alkylation of the Heavy Elements* 1987, The Royal Society of Chemistry, London, UK.
2. IPCS *Environmental Health Criteria* No. 116: Tributyltin Compounds 1990, WHO, Geneva, Switzerland.
3. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
5. S. I. 1987, No. 783 *Control of Pollution (Anti-Fouling Paints and Treatments) Regulations* 1987, HMSO, London, UK.
6. Tanaka, H. et al *Bokin Bobai* 1987, 15(1), 11-22 (Japan.) (*Chem. Abstr.* 106, 209333n).
7. Thayer, J. S. et al *Adv. Organomet. Chem.* 1982, 20, 313.
8. Thompson, J. A. J. et al *Organotin Compounds in the Aquatic Environment* 1985, National Research Council Canada, Assoc. Comm. Sci. Criteria Environ. Qual. Publ. No. NRCC2294.
9. Byrne, C. D. *Selection of Substances Requiring Priority Action* in Richardson, M. L. (Ed.) *Risk Assessment of Chemicals in the Environment* 1988, 414-436, The Royal Society of Chemistry, London, UK

T221 tributyltin succinate



$\text{C}_{28}\text{H}_{58}\text{O}_4\text{Sn}_2$

Mol. Wt. 696.19

CAS Registry No. 4644-96-6

Synonyms bis(tributyltin) succinate; bis(tri-*n*-butyltin) succinate; [(1,4-dioxo-1,4-butanediyl)bis(oxy)]-bis(tributylstannane); (succinyldioxy)bis(tributylstannane); bis(tributyltin) succinate

Uses Antifouling agent. Polymerisation catalyst.

Physical properties

M. Pt. 91-98.5°C

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Sn) (total dust)

SE-LEVL 0.1 mg m⁻³ (as Sn)

SE-STEL 0.2 mg m⁻³ (as Sn)

UK-LTEL 0.1 mg m⁻³ (as Sn)

UK-STEL 0.2 mg m⁻³ (as Sn)

US-TWA 0.1 mg m⁻³ (as Sn)

US-STEL 0.2 mg m⁻³ (as Sn)

UN No. 2788 (liquid); 3146 (solid) HAZCHEM Code 2X (solid) **Conveyance classification** toxic substance

Supply classification toxic

Risk phrases Harmful in contact with skin – Toxic if swallowed – Irritating to eyes and skin – Toxic: danger of serious damage to health by prolonged exposure through inhalation and if swallowed (R21, R25, R36/38, R48/23/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – This material and its container must be disposed of in a safe way – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S35, S36/37/39, S45)

Environmental fate

Degradation studies

Organotins can be degraded by light, but light may also stimulate photosynthetic organisms which carry out degradation (1).

Mammalian & avian toxicity

Irritancy

Tributyltin compounds are irritants to the skin and eyes; inhalation of aerosols leads to respiratory irritation (2).

Other effects

Any other adverse effects

In experimental animals, tributyltin compounds cause damage to the liver, haematological and endocrine systems, and are irritating to the skin and eyes. Inhalation of aerosols leads to respiratory irritation (2).

Adverse effects to the immune system in rats have been reported. The no-observed-effect level for tributyltin compounds using the *Trichinella spiralis* host-resistance model in rats 0.5-5.0 mg kg⁻¹ diet (2).

Legislation

Included in Schedules 5 and 6 (Release into Water and Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (3).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (4).

Included in Control of Pollution (Anti-Fouling Paints and Treatments) Regulations 1987 (5).

Other comments

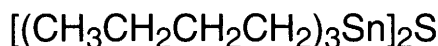
Exposure of workers to tributyltin compounds occurs mainly in the manufacture, application and removal of tributyltin paints and wood preservatives. Exposure of the general public may arise from the contamination of food, particularly fish and shellfish, and from domestic applications of wood preservatives (2).

Toxicity of tributyltin compounds reviewed (2,6-8).

References

1. Craig, P. J. (Ed.) *The Biological Alkylation of Heavy Elements* 1987, The Royal Society of Chemistry, London, UK.
2. *IPCS Environmental Health Criteria No. 116: Tributyltin Compounds* 1990, WHO, Geneva, Switzerland.
3. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
5. S. I. 1987, No. 783 *Control of Pollution (Anti-Fouling Paints and Treatments) Regulations* 1987, HMSO, London, UK.
6. Thayer, J. S. et al *Adv. Organomet. Chem.* 1982, **20**, 313.
7. Thompson, J. A. J. et al *Organotin Compounds in the Aquatic Environment* 1985, National Research Council Canada, Assoc. Comm. Sci. Criteria Environ. Qual. Publ. No. NRCC2294.
8. Byrne, C. D. *Selection of Substances Requiring Priority Action* in Richardson, M. L. (Ed.) *Risk Assessment of Chemicals in the Environment* 1988, 414-436, The Royal Society of Chemistry, London, UK

T222 tributyltin sulfide



$\text{C}_{24}\text{H}_{54}\text{SSn}_2$

Mol. Wt. 612.18

CAS Registry No. 4808-30-4

Synonyms 1,1,1,3,3,3-hexabutylstannathiane; hexabutylstannathiane; bis(tributyltin) sulfide

EINECS No. 225-369-7

RTECS No. JN 8830000

Uses Antifouling agent. Polymerisation catalyst.

Occurrence Has been detected in sediments (1).

Physical properties

B. Pt. 186°C at 0.02 mmHg

Occupational exposure

DE-MAK 0.1 mg m^{-3} (as Sn) (total dust)

SE-LEVL 0.1 mg m^{-3} (as Sn)

SE-STEL 0.2 mg m^{-3} (as Sn)

UK-LTEL 0.1 mg m^{-3} (as Sn)

UK-STEL 0.2 mg m^{-3} (as Sn)

US-TWA 0.1 mg m^{-3} (as Sn)

US-STEL 0.2 mg m^{-3} (as Sn)

UN No. 2788 (liquid); 3146 (solid) **HAZCHEM Code** 2X (solid) **Conveyance classification** toxic substance

Supply classification toxic

Risk phrases Harmful in contact with skin – Toxic if swallowed – Irritating to eyes and skin – Toxic: danger of serious damage to health by prolonged exposure through inhalation and if swallowed (R21, R25, R36/38, R48/23/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – This material and its container must be disposed of in a safe way – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S35, S36/37/39, S45)

Ecotoxicity

Invertebrate toxicity

Rhithropanopeus harrisii exposed to $\geq 20 \mu\text{g l}^{-1}$, sublethal responses observed (2).

Environmental fate

Degradation studies

Organotins can be degraded by light, but light may also stimulate photosynthetic organisms which carry out degradation (3).

Mammalian & avian toxicity

Acute data

LD_{Lo} oral mouse 470 mg kg⁻¹ (4).

LD₅₀ intraperitoneal mouse 140 mg kg⁻¹ (5).

Other effects

Any other adverse effects

In experimental animals, tributyltin compounds cause damage to the liver, haematological and endocrine systems, and are irritating to the skin and eyes. Inhalation of aerosols leads to respiratory irritation (6).

Adverse effects to the immune system in rats have been reported. The no-observed-effect level for tributyltin compounds using the *Trichinella spiralis* host-resistance model in rats was 0.5-5.0 mg kg⁻¹ diet (6).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 $\mu\text{g l}^{-1}$ (7).

Included in Schedules 5 and 6 (Release into Water and Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (8).

Included in US EPA TSCA Chemical Inventory, June 1990 (9).

Included in Control of Pollution (Anti-Fouling Paints and Treatments) Regulations 1987 (10).

Other comments

Exposure of workers to tributyltin compounds occurs mainly in the manufacture, application and removal of tributyltin paints and wood preservatives. Exposure of the general public may arise from the contamination of food, particularly fish and shellfish, and from domestic applications of wood preservatives (6).

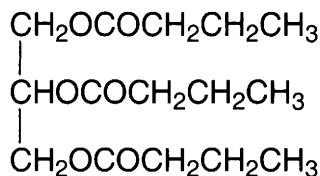
Toxicity of tributyltin compounds reviewed (1,6,11,12).

References

1. Byrne, C. D. *Selection of Substances Requiring Priority Action* in Richardson, M. L. (Ed.) *Risk Assessment of Chemicals in the Environment* 1988, 414-436, The Royal Society of Chemistry, London, UK.
2. Langhlin, R. et al *Water Air Soil Pollut.* 1983, **20**(1), 69-79.
3. Craig, P. J. (Ed.) *The Biological Alkylation of Heavy Elements* 1987, The Royal Society of Chemistry, London, UK.
4. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1985, **14**, 111.
5. Russ. *Pharmacol. Toxicol.* 1979, **42**, 73.

6. *IPCS Environmental Health Criteria No. 116 Tributyltin Compounds* 1990, WHO, Geneva, Switzerland.
7. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
8. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
9. National Institute for Occupational Safety and Health, *RTECS Register* October 1990.
10. *S. I. 1987, No. 783 Control of Pollution (Anti-Fouling Paints and Treatments) Regulations* 1987, HMSO, London, UK.
11. Thayer, J. S. et al *Adv. Organomet. Chem.* 1982, **20**, 313.
12. Thompson, J. A. J. et al *Organotin Compounds in the Aquatic Environment* 1985, National Research Council Canada, Assoc. Comm. Sci. Criteria Environ. Qual. Publ. No. NRCC2294

T223 tributyrin



$\text{C}_{15}\text{H}_{26}\text{O}_6$

Mol. Wt. 302.37

CAS Registry No. 60-01-5

Synonyms butyrin; tributryl glyceride; butyryl triglyceride; glyceryl tributryate; 1,2,3-propanetriyl butanoate; tributrin; tri-*n*-butyrin

EINECS No. 200-451-5

RTECS No. ET 7350000

Uses Flavour agent. Solvent. Plasticiser.

Physical properties

M. Pt. -75°C **B. Pt.** $287-288^\circ\text{C}$ **Flash point** 173°C **Specific gravity** 1.0356 at 20°C with respect to water at 20°C

Solubility Organic solvents: acetone, benzene, chloroform, diethyl ether, ethanol

Environmental fate

Degradation studies

Hydrolysed by several strains of *Branhamella catarrhalis*, *Neisseria caviae*, *Neisseria cuniculi* and *Neisseria ovis* (1).
Biodegradation by activated sludge process involves stepwise hydrolysis to give butyric acid (2).

Mammalian & avian toxicity

Acute data

Inhalation rat (6 hr) 78 ppm caused temporary hypernoea (3).

LD_{50} oral rat, mouse 3200, 13,000 mg kg^{-1} , respectively (4,3).

LD_{50} intravenous mouse 320 mg kg^{-1} (5).

Carcinogenicity and chronic effects

Oral rat (35 wk) 15-25% in diet. 30/113 animals died in the first week of the study. Animals surviving to necropsy showed hyperplasia, hyperkeratosis, papillomatosis, acanthosis, infiltration and occasional ulceration. Cysts were observed in the glandular stomach of some animals (6).

Metabolism and toxicokinetics

Hydrolysed by some lung esterases and by mammalian microsomal esterases (3,7).

Other effects

Any other adverse effects

Oral mouse 12% diet increased butyrylcholinesterase activity to $\sim 2.4 \times$ normal and reduced acetylcholinesterase activity to $\sim 0.55 \times$ normal levels (8).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (9).

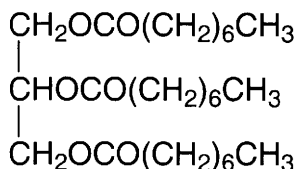
Other comments

Autoignition temperature 410°C.

References

1. Riley, T. V. J. *Appl. Bacteriol.* 1987, **62**(6), 539-542.
2. Niitsuma, T. et al *Tohoku Gakuin Daigaku Kogakubu Kerkyu Hokoku* 1988, **23**(1), 65-68 (Japan.) (*Chem. Abstr.* **110**, 159777v).
3. *Patty's Industrial Hygiene and Toxicology* 3rd ed., 1981, **2A**, 2323, Wiley Interscience, New York, NY, USA.
4. *Kodak Company Reports* 1971, Rochester, NY, USA.
5. *Acta Physiol. Scand.* 1957, **40**, 338.
6. *J. Natl. Cancer Inst.* 1949, **10**, 361.
7. *Naunyn-Schmiedeberg's Arch. Pharmacol. Exp. Pathol.* 1966, **255**(2), 163.
8. Mezinceso, M. D. et al *Biochem. Biophys. Acta* 1974, **350**(1), 54.
9. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T224 tricaprylin



$\text{C}_{27}\text{H}_{50}\text{O}_6$

Mol. Wt. 470.69

CAS Registry No. 538-23-8

Synonyms caprylic acid triglyceride; glycerin tricaprylate; tricaprylate; octanoic acid triglyceride; Panacet 800; RATO; Sefsol 810; tricaprylic glyceride

EINECS No. 208-686-5

RTECS No. YJ 7700000

Physical properties

M. Pt. 10°C B. Pt. 223°C **Specific gravity** 0.9540 at 20°C with respect to water at 4°C

Solubility Organic solvents: acetone, benzene, diethyl ether, ethanol, light petroleum, ligroin

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 29, 33 g kg⁻¹, respectively (1).

LD_{Lo} intraperitoneal rabbit 3400 mg kg⁻¹ (2).

LD₅₀ intravenous rat 4 g kg⁻¹ (1).

LD₅₀ intravenous mouse 3700 mg kg⁻¹ (3).

Teratogenicity and reproductive effects

Oral rat, lowest toxic dose 250 g kg⁻¹ day⁻¹ on 7th day prior to mating through to day 21 of gestation (parameters investigated were growth statistics and weaning index) (4).

Gavage mouse 4750 mg kg⁻¹ day⁻¹ on days 7-15 of gestation did not cause any significant maternal, foetotoxic or teratogenic effects (5).

Metabolism and toxicokinetics

Hydrolysed to yield octanoic acid by human fibroblasts and lymphoblasts *in vitro* (6).

Following intravenous administration of 100 or 300 mg kg⁻¹ to fasted rabbits, ketone bodies in the blood peaked after 120-180 min (7).

Other effects

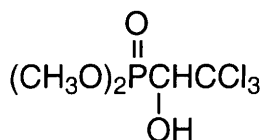
Any other adverse effects

In vivo rat liver foci bioassay positive (8).

References

1. *Oyo Yakuri* 1970, **4**, 871.
2. *J. Natl. Cancer Inst.* 1975, **54**, 1439.
3. *Acta Physiol. Scand.* 1957, **40**, 332.
4. *Iyakuhiin Kenkyu* 1972, **3**, 180.
5. Hardin, B. D. *Teratog., Carcinog., Mutagen.* 1987, **7**(1), 29-48.
6. Lemmen, P. et al *Biol. Chem. Hoppe-Leyler* 1988, **369**(12), 1267-1273.
7. Hioki, T. et al *Nippon Jomyaku, Keicho Eitoy Kenkyukaishi* 1988, **3**, 244-247 (Japan.) (*Chem. Abstr.* **110**, 21519f).
8. Herren-Freund, S. L. et al *Environ. Health Perspect.* 1986, **69**, 59-65

T225 trichlorfon



C₄H₈Cl₃O₄P

Mol. Wt. 257.44

CAS Registry No. 52-68-6

Synonyms *O,O*-dimethyl-1-hydroxy-2,2,2-trichloroethyl phosphonate; dimethyl 2,2,2-trichloro-1-hydroxyethylphosphonate; DEP; DETP; Dimetox; Diparex; Detrofon; Foschlor; Hypodermacid; Masoten; methyl chlorofos; Metrifonate; Neguron; Phoschlor; Votexit

EINECS No. 200-149-3

RTECS No. TA 0700000

Uses Insecticide. Veterinary anthelmintic.

Physical properties

M. Pt. 78.5°C, delayed melting to 84°C **B. Pt.** 100°C at 0.1 mmHg **Specific gravity** 1.73 at 20°C with respect to water at 4°C **Partition coefficient** log P_{ow} 0.43 at 20°C **Volatility** v.p. 7.8 × 10⁶ mmHg at 20°C **Solubility** Water: 154 g l⁻¹ at 25°C. Organic solvents: acetone, benzene, chloroform, dichloromethane, diethyl ether, hexane, pentane, toluene

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed – May cause sensitisation by skin contact (R22, R43)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with the skin – Wear suitable gloves (S2, S24, S37)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bluegill sunfish, golden orfe, rainbow trout 0.26, 52, 0.7 mg l⁻¹, respectively (1,2,3).

LC₅₀ (96 hr) carp 14 mg l⁻¹ (2).

Invertebrate toxicity

LC₅₀ (48 hr) *Daphnia pulex* 0.18 µg l⁻¹ (4).

LC₅₀ (96 hr) *Gammarus lacustris* 40 µg l⁻¹ (5).

LD₅₀ topical bee 2.29 µg bee⁻¹ (6).

Environmental fate

Degradation studies

Complete biodegradation in river water occurred within 5 days at 10 mg kg⁻¹, 13 days at 20 mg l⁻¹, and 20 days at 30 mg l⁻¹ (7).

Persistence in soils ≤2 wk. Degraded by ammonifying microorganisms (8).

Degraded by nitrogen fixation, microorganisms of the host plants *Rhizobium leguminosarum* and *Rhizobium trifolii* (9).

Abiotic removal

UV irradiation yields dichlorvos and a number of other products, including O-methyl-2,2-dichlorovinyl phosphate, dichlorovinyl alcohol, dichloroacetaldehyde, dichloroacetic acid and 2,2-dichloroethanol (10,11).

Undergoes hydrolysis and dechlorination (1).

Adsorption and retention

Adsorption by soils 0.3-1.5 g kg⁻¹ (12).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird, starling 37-75 mg kg⁻¹ (13,14).

LD₅₀ oral rabbit, rat, mouse 160, 250, 300 mg kg⁻¹, respectively (15,16).

LC₅₀ (4 hr) inhalation rat >500 mg m⁻³ (17).

LD₅₀ dermal rat 2000 mg kg⁻¹ (17).

LD₅₀ subcutaneous mouse, rat 270, 400 mg kg⁻¹, respectively (18,19).

LD₅₀ intraperitoneal rat, mouse 160, 200 mg kg⁻¹, respectively (20,21).

LD₅₀ intravenous mouse 290 mg kg⁻¹ (22).

Sub-acute and sub-chronic data

LC₅₀ (5 day) oral bobwhite quail, Japanese quail, pheasant 720-3400 mg kg⁻¹ diet (23).

Single dose of 140, 250 or 350 mg kg⁻¹ to rats (route unspecified) caused dose-related effects on haemoglobin concentration and the number of erythrocytes, leukocytes and blood platelets. Sperm motility and ovarian cycle were also affected. The effects were noticeable for 1-2 months after administration (24).

Oral rat, 300 mg kg⁻¹ day⁻¹ for 5 days caused brain oedema, congestion of organs, fatty degeneration and glycogen depletion in the liver and in the heart muscle, emphysema and local inflammation in the lungs (25).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (26).

Oral mice 900 or 2700 mg kg⁻¹ in the diet for 2 yr. Body weights were significantly increased in mice given 2700 mg kg⁻¹, and liver weights were increased in ♀ mice given 900 and 2700 mg kg⁻¹. All treated groups showed a dose-related decrease in blood cholinesterase activity. No compound-related tumorigenicity was found (27).

Gavage rat, mouse (2 yr) 30 and 22 mg kg⁻¹, respectively, 2 × wk⁻¹ caused no significant difference in cancer incidence compared with controls (28,29).

Intraperitoneal rats (118 wk) 12 mg kg⁻¹ 2 × wk⁻¹ for 90 wk; mice (80 wk) 28 mg kg⁻¹ 2 × wk⁻¹ for 75 wk; and intraperitoneal hamsters (100 wk) 20 mg kg⁻¹ wky for 90 wk. There was no significant difference in the incidence of tumours between controls and treated animals (28-30).

Dermal mouse, 15 mg kg⁻¹ 2 × wk⁻¹ for 6 wk, they were then observed for life. 5/14 treated mice developed malignant tumours (myeloid leukaemia) within 406 days. Control data were unavailable (31).

Dermal mouse (80 wk) 0.25 ml of 1% solution 2 × wk⁻¹ for 75 wk (cumulative dose 375 mg). There was no significant difference in the incidence of tumours between treated animals and controls (29).

Subcutaneous rats 15 mg kg⁻¹ 2 × wk⁻¹ for life. The average survival time was 1711 days for controls and 565 days for treated rats. 4/27 treated rats developed malignant tumours in several organs compared with 0/35 in controls, and 7/27 benign tumours were reported in treated rats compared with 4/35 controls (31).

Teratogenicity and reproductive effects

Gavage mouse 300, 400, 500 or 600 mg kg⁻¹ day⁻¹ on days 10-14 of gestation. The two highest doses caused reduced food intake and body-weight gain in dams, reduced foetal weight and a slight but significant increase in the incidence of cleft palate (32).

Inhalation rat, 0.005, 0.02, 0.2 or 9 mg m⁻³ throughout gestation. No teratogenic effects or changes in placental history occurred (33).

In a three-generation study, rats administered 60 mg kg⁻¹ day⁻¹ in drinking water produced progeny with reduced viability and body weight (34).

Metabolism and toxicokinetics

Following dermal and gavage administration to cows, trichlorfon and dichlorvos were detected in the milk for up to 22 days (10).

Readily absorbed from gastro-intestinal tract following oral administration of 7.5 mg kg⁻¹ to human volunteers. Trichlorfon, and its rearrangement product dichlorvos, were detected in the blood. Whole blood t_{1/2} for trichlorfon ~3 hr (35).

Following oral administration to mice, metabolites detected in the urine included dimethyl phosphoric acid, dichlorvos and monomethyl phosphoric acid (36).

Following intraperitoneal administration to rats, urinary metabolites included dimethyl phosphate (35.7%), phosphoric acid (0.8%), methyl phosphate (0.8%), O-demethyltrichlorfon (1.4%), O-demethyldichlorvos (0.8%) and unmetabolised trichlorfon (0.7%) (37).

Irritancy

120 mg instilled into rabbit eye intermittently for 6 days caused mild irritation (38).

Sensitisation

Allergic dermatitis had been frequently reported among workers exposed to trichlorfon and dicofol (10).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537, TA1538 with and without metabolic activation positive (39,40).

Escherichia coli SOS chromotest with and without metabolic activation negative (41).

Saccharomyces cerevisiae D7 mitotic crossing over and gene conversion with and without metabolic activation positive (42).

Drosophila melanogaster sex-linked recessive lethal assay and gene mutation negative (43).

In vitro mouse lymphoma L5178Y cells tk⁺/tk⁻ forward mutation assay positive (44).

In vitro human epithelium cells, unscheduled DNA synthesis positive (45).

In vitro Chinese hamster ovary and V79 cells sister chromatid exchanges positive (42,46,47).

Did not induce micronuclei *in vivo* in mouse bone marrow cells (42,47).

In vivo mouse bone marrow cells chromosomal aberrations positive (48).

Chromatid-type aberrations in peripheral lymphocytes were reported to have increased in exposed factory workers (49).

In vivo mouse dominant lethal assay positive (50).

Other effects

Other adverse effects (human)

Changes in functional state of the central nervous system were demonstrated by EEG spectrum patterns in exposed workers (51).

Any other adverse effects

Intramuscular rat, single dose of 80 mg kg⁻¹ reduced brain cholinesterase activity to 26% at 30 min recovered to 50% at 180 min and to 79% at 300 min. Levels of acetylcholine increased by 45% at 45 min, then returned to normal by 120 min. When administered intraventricularly (2.5 mg) cholinesterase activity decreased at 30 min to 20% in the hippocampus, 22% in the medulla, 50% in the cerebellum, 58% in the striatum and to 72% in the cortex. Levels of acetylcholine increased maximally at 45 min in the hippocampus and cortex and peaked in the striatum at 60 min (52).

Intraperitoneal rat, single dose of 150 mg kg⁻¹ doubled the activities of superoxide dismutase and microsomal cytochrome P₄₅₀, and caused a 1.4-fold increase in lipid peroxidation in the liver within 150 min (53).

The acute toxicity of trichlorfon is due to inhibition of acetylcholinesterase at nerve endings, leading to an accumulation of endogenous acetylcholine. The effects are manifested by muscarinic, narcotic and central nervous system signs and symptoms: sweating, salivation, diarrhoea, bronchorrhea, bradycardia, bronchoconstriction, muscle fasciculations and coma. The cause of death is primarily respiratory failure (54).

Legislation

EEC maximum residue levels: cereals 0.1 ppm; fruit and vegetables 0.5 ppm (1).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (55).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (56).

WHO Toxicity Class III (57).

EPA Toxicity Class II (formulation) (3).

ADI (JMPR) 0.01 mg kg⁻¹ body weight (3).

Other comments

A racemate consisting of a 1:1 mixture of the (1R) and (1S) enantiomers.

A minor ingredient of coumaphos. Residues have been isolated from water, sediments, soil, animal tissues and crops (58,59).

Physical properties, use, occurrence, carcinogenicity, mammalian toxicity, teratogenicity, metabolism and mutagenicity reviewed (10,59).

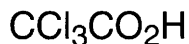
Trichlorfon is reported to be effective in the treatment of schistosomiasis in humans (60).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. Neubert, J. *Acta Hydrochim. Hydrobiol.* 1986, **14**(6), 643-651, (Ger.) (*Chem. Abstr.* **106**, 97726j).
3. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
4. Sanders, H. O. *The Toxicities of Some Insecticides to Four Species of Malacostracan Crustacea* 1972, Fish Pesticide Residue Laboratory, Bureau of Sport, Fish and Wildlife, Columbia, MO, USA.
5. Sanders, H. O. *Toxicity of Pesticides to the Crustacean Gammarus lacustris* 1969, Bureau of Sport, Fisheries and Wildlife, Technical Paper 25, Govt. Printing Office, Washington, DC, USA.
6. Nijima, K. et al *Tamagawa Daigaku Nogakubu Kerkyu Hokoku* 1985, (25), 83-90 (Japan.) (*Chem. Abstr.* **106**, 14397d).
7. Zdyliewska, M. W. *Przem. Chem.* 1988, **67**(8), 378-379 (Pol.) (*Chem. Abstr.* **109**, 196461n).
8. Molozhanova, E. G. et al *Khim. Sel. Khz.* 1973, **11**, 761-762 (Russ.) (*Chem. Abstr.* **80**, 116858s).
9. Salma, A. M. et al *Acta Biol. Acad. Sci. Hyg.* 1975, **26**, 1-7 (*Chem. Abstr.* **84**, 85567x).
10. *IARC Monograph* 1983, **30** 207-231.
11. Giovanoli-Jakubxyak, T. et al *Rocz. Chem.* 1971, **45** 689-694.
12. Muzychuk, N. T. et al *Gig. Sanit.* 1988, (11), 85-86 (Russ.) (*Chem. Abstr.* **110**, 35051j).
13. Schafer, E. W. *Toxicol. Appl. Pharmacol.* 1972, **21**, 315-330.

14. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
15. *Farm Chemicals Handbook* 1989, **C294**, Meister Publ., Willoughby, OH, USA.
16. *Special Publication of the Entomological Society of America* 1974, 74-1.
17. *Arch. Geschwulstforsch.* 1978, **48**, 12.
18. *Arzneim.-Forsch.* 1981, **31**, 555.
19. *J. Econ. Entomol.* 1957, **50**(3), 356.
20. *Advance. Pest Control Res.* 1961, **4**, 117.
21. *Toxicol. Appl. Pharmacol.* 1960, **2**, 495.
22. *Arch. Toxicol.* 1978, **41**, 3.
23. Hill, E. W. et al *Lethal Dietary Toxicities of Environmental Pollutants to Birds* 1975, US Fish and Wildlife Service, Report Wildlife No. 191, Washington, DC, USA.
24. Pintsckhalava, A. V. *Izv. Akad. Nauk Gruz. SSR. Len. Biol.* 1990, **16**(3), 161-165 (Russ.) (*Chem. Abstr.* **114**, 158803w).
25. Karmilov, V. A. *Farmakol. Toksikol.* 1973, **36**, 727-728.
26. *IARC Monograph* 1987, **Suppl.** 7, 73.
27. Hayes, R. H. (Bayer AG) *Oncogenicity Study of Technical Grade Trichlorfon with Mice* 1988, Proprietary Study Report No. 1039 submitted to WHO, Geneva, Switzerland.
28. Deichmann, B. et al *Arch. Geschwulstforsch.* 1978, **48**, 310-307.
29. Deichmann, B. et al *Arch. Geschwulstforsch.* 1978, **48**, 112-119.
30. Deichmann, B. et al *Arch. Geschwulstforsch.* 1978, **48**, 718-721.
31. Gibel, V. W. et al *Arch. Geschwulstforsch.* 1973, **41**, 311-328.
32. Staples, R. E. et al *Environ. Health Perspect.* 1979, **30**, 105-113.
33. Gofmekler, V. A. et al *Farmakol. Toksikol.* 1970, **33**, 735-737.
34. Rybak, M. *Rocz. Panstw. Zakl. Hig.* 1973, **24**, 465-475.
35. Abdi, Y. A. et al *Pharmacol. Toxicol. (Copenhagen)* 1991, **68**(2), 137-139.
36. Miyata, T. et al *Botyu-Kogaku* 1973, **38**, 81-86.
37. Bull, D. L. et al *J. Agric. Food Chem.* 1969, **17**, 837-841.
38. *Bull. Univ. Miami Sc. Med. Jackson Mem. Hosp.* 1955, **9**, 7.
39. Klopman, G. et al *Mutat. Res.* 1990, **228**, 1-50.
40. Barrueco, C. et al *Mutagenesis* 1991, **6**(1), 71-76.
41. Xu, H. H. et al *Toxic. Assess.* 1990, **5**(1), 1-14.
42. Jones, D. C. L. et al *In Vitro Mutagenicity Studies of Environmental Chemicals* 1982, NTIS, Washington DC, USA.
43. Waters, M. D. et al *J. Environ. Sci. Health* 1980, **B15**, 867-906.
44. McGregor, D. B. et al *Environ. Mol. Mutagen.* 1988, **12**(1), 85-154.
45. Benigni, R. et al *Mutat. Res.* 1980, **74**, 217.
46. Chen, H. H. et al *Mutat. Res.* 1981, **88**, 307-316.
47. Waters, M. D. et al in *Genetic Toxicology An Agricultural Perspective* Fleck, R. et al (Eds.) 1982, Plenum Press, NY, USA.
48. Ryazanova, R. A. et al *Gig. Sanit.* 1980, **1**, 80-81.
49. Kivaly, J. et al *Mutat. Res.* 1977, **46**, 224.
50. Schiemann, S. *Wiss. Z. Martin Luther Univ., Halle Wittenbergs, Math.-Naturwiss. Reihe* 1975, **24**, 85-86.
51. Povorinskii, A. G. et al *Gig. Tr. Prof. Zabol.* 1990, (3), 28-31 (Russ.) (*Chem. Abstr.* **113**, 217203e).
52. Hallak, M. et al *Neuropharmacology* 1987, **26**(6), 521-530.
53. Matkovics, B. et al *Gen. Pharmacol.* 1980, **11**, 353-356.
54. Goodman L. S. et al (Eds.) *The Pharmacological Basis of Therapeutics* 6th, ed., 1980, 100-110, MacMillan, New York, NY, USA.
55. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
56. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
57. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
58. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
59. *IPCS Environmental Health Criteria No. 132: Trichlorfon* 1992, WHO, Geneva, Switzerland.
60. Nordgmen, I. et al *Curr. Res. Alzheim. Ther: Cholinesterase Inhib.* 1988, 281-288.

T226 trichloroacetic acid



$\text{C}_2\text{HCl}_3\text{O}_2$

Mol. Wt. 163.39

CAS Registry No. 76-03-9

Synonyms TCA; 1,1,1-trichloroethanoic acid; Antigam 95 GR; Antyperz; Calliact; Dozer; Konesta; Roan

EINECS No. 200-927-2

RTECS No. AJ 7875000

Uses Herbicide, in combination with 2,4-D or dalapon. Decalcifier and fixative in microscopy. Protein precipitant. Organic synthesis. Removal of tattoos and warts.

Physical properties

M. Pt. 54-56°C **B. Pt.** 196°C **Flash point** >110°C **Specific gravity** 1.6298 at 61°C with respect to water at 4°C

Partition coefficient $\log P_{\text{ow}}$ 0.10/1.96 (calc.) (1) **Volatility** v.p. 1 mmHg at 51°C

Solubility Water: 1g in 0.1 ml. Organic solvents: miscible with diethyl ether, ethanol

Occupational exposure

FR-VME 1 ppm (5 mg m⁻³)

US-TWA 1 ppm (6.7 mg m⁻³)

UN No. 1839

UN No. 2564 (solution) **HAZCHEM Code** 2X **Conveyance classification** corrosive substance

Supply classification corrosive

Risk phrases Causes severe burns (R35)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Avoid contact with skin and eyes – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S24/25, S26, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow 2000 mg l⁻¹ (sodium salt) (2).

Invertebrate toxicity

LC₅₀ (48 hr) *Daphnia magna* 2000 mg l⁻¹ (sodium salt) (2).

Toxicity threshold (cell multiplication test) *Pseudomonas putida* >1000 mg l⁻¹, *Scenedesmus quadricauda* 200 mg l⁻¹, *Entosiphon sulcatum* 800 mg l⁻¹ (3).

Environmental fate

Anaerobic effects

IC₅₀ (50 day) methanogenic bacterial culture <1 µg l⁻¹ (4).

Degradation studies

Degraded by species of *Pseudomonas*, *Anthrobacter* and the fungus *Trichoderma viride* (5).

Abiotic removal

Aqueous concentrations of <30% strength spontaneously decompose to form chloroform, hydrochloric acid, carbon dioxide and carbon monoxide (6).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 400 mg kg⁻¹ (pure); 3200-5000 mg kg⁻¹ (sodium salt) (7,8).

LD₅₀ subcutaneous mouse 270 mg kg⁻¹ (9).

LD_{Lo} intraperitoneal mouse 500 mg kg⁻¹ (10).

Sub-acute and sub-chronic data

Oral rat 0.3 or 3.0 g l⁻¹ in drinking water for 3 wk. The highest dose caused a decrease in body-weight gain, which was attributed to a reduction in water intake. Kidney function was not impaired (11).

Carcinogenicity and chronic effects

♂ Mice were administered 0, 2.5 or 10 µg g⁻¹ *N*-ethyl-*N*-nitrosourea on day 15 of age. At 28-days-old the mice were given 2 or 5 g trichloroacetic acid l⁻¹ in drinking water for 61 wk. Concentrations of 5 g trichloroacetic acid l⁻¹ were carcinogenic without prior initiation of *N*-ethyl-*N*-nitrosourea, with 32% of animals developing hepatocellular carcinomas (12).

Teratogenicity and reproductive effects

Intraperitoneal ♂ mouse lowest toxic dose 125 mg kg⁻¹ administered 5 days prior to mating affected spermatogenesis (13).

Oral rat lowest foetotoxic dose 3300 mg kg⁻¹ day⁻¹ on days 6-15 of gestation. Doses of 8000 mg kg⁻¹ caused foetal deaths (14).

Irritancy

Dermal rabbit 210 µg caused mild irritation (exposure unspecified) (15).

3.5 mg instilled into rabbit eye for 5 sec caused severe irritation (15).

Genotoxicity

Escherichia coli PQ 37 SOS chromotest negative (16).

Salmonella typhimurium TA100 Ames fluctuation test positive (16).

Newt micronucleus assay detected a weak clastogenic effect on the peripheral blood erythrocytes of *Pleurodeles waltl* larvae (16).

A Computer Automated Structure Evaluation (CASE) predicted marginal activity in *Salmonella typhimurium* TA97, TA98, TA100, TA1535, TA1537 and TA1538 (17).

In vivo mouse bone marrow chromosomal aberrations, micronuclei and sperm-head abnormality positive (18).

Other effects

Other adverse effects (human)

Inhalation may be fatal as a result of spasm, inflammation and oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema (19).

Legislation

WHO guideline value for drinking water 100 µg l⁻¹ (provisional) (20).

Other comments

Disinfection by-product in chlorinated waters (20,21).

Trichloroacetic acid is a metabolite of trichloroethylene and is thought to contribute to its hepatocarcinogenic effects in mice (22).

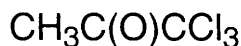
Physical properties, use, toxicity and safety precautions reviewed (23,24).

References

1. Vershueren, K. *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, 1120, Van Nostrand Reinhold, New York, NY, USA.
2. Williams, H. D. *Environ. Sci. Technol.* 1979, 13(5), 594-598.

3. Bringmann, G. et al *Water Res.* 1980, **14**, 231-241.
4. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, **63**(3), 198-207.
5. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
6. Kearney, P. C. et al (Eds.) *Herbicides: Chemistry, Degradation and Mode of Action* 2nd ed., 1975, 416, Marcel Dekker, New York, NY, USA.
7. Bailey, G. W. et al *Res. Rev.* 1965, **10**, 97.
8. *The Pesticide Manual* 10th ed., 1994, British Crop Protection Council/The Royal Society of Chemistry, Cambridge, UK.
9. *Drugs in Japan. Ethical Drugs* 6th ed., 1982, 879, Jukgyo Jiho Co., Tokyo, Japan.
10. *Summary Tables of Biological Tests* 1982, **6**, 879, National Research Council Chemical-Biological Coordination Center, Washington, DC, USA.
11. Davies, M. E. *Environ. Health Perspect.* 1986, **69**, 209-214.
12. Herren-Freund, S. L. et al *Toxicol. Appl. Pharmacol.* 1987, **90**, 183-189.
13. *Mutat. Res.* 1987, **188**, 215.
14. *Teratology* 1989, **40**, 445.
15. *Report No. MDCC-01715* Atomic Energy Commission, Univ. Rochester, New York, NY, USA.
16. Giller, S. et al *Mutagenesis* 1997, **12**(5), 321-328.
17. Klopman, G. et al *Mutat. Res.* 1990, **228**, 1-50.
18. Bhunya, S. P. et al *Mutat. Res.* 1987, **188**, 215-221.
19. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3402, Sigma-Aldrich, Milwaukee, WI, USA.
20. *Guideline values for Drinking Water Quality* 2nd ed., 1993, **1**, WHO, Geneva, Switzerland.
21. Comes, R. D. et al *Weed Sci.* 1975, **23**(3), 207-210.
22. Stenner, R. D. et al *Drug Metab. Dispos.* 1997, **25**(5), 529-535.
23. *Chemical Safety Data Sheets* 1990, **3**, 264-266, The Royal Society of Chemistry, London, UK.
24. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels

T227 1,1,1-trichloroacetone



$\text{C}_3\text{H}_3\text{Cl}_3\text{O}$

Mol. Wt. 161.41

CAS Registry No. 918-00-3

Synonyms 1,1,1-trichloro-2-propanone; α,α,α -trichloroacetone; 1,1,1-trichloropropanone

RTECS No. UC 3839000

Physical properties

B. Pt. 134-135°C Flash point 64°C Specific gravity 1.435

Mammalian & avian toxicity

Carcinogenicity and chronic effects

Dermal mice (24 wk) 400, 600 or 800 mg kg⁻¹ in ethanol 6 × over 2 wk. Two wk later animals received 1 µg 12-*o*-tetradecanoylphorbol-13-acetate topically 3 × wk⁻¹ for 20 wk. At the end of the study skin papillomas were seen in 3/30, 2/40 and 0/40 mice in the low, medium and high dose groups, respectively (1).

Oral mice (24 wk) total dose of 600 or 900 mg kg⁻¹, then treated topically as above. Skin papillomas were seen in 0/29 and 2/39 mice, respectively (1).

Teratogenicity and reproductive effects

No effects were seen in the incidence of sperm with head-shape abnormalities, testis weight or epididymal sperm concentration in mice 21 or 35 days after treatment (2).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535 with and without metabolic activation positive (3).
In vitro Chinese hamster ovary cells with and without metabolic activation chromosomal aberrations positive (2).
In vivo mice bone marrow cells no increase in micronucleated polychromatic erythrocytes (2).

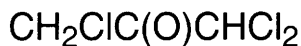
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level 1 $\mu\text{g l}^{-1}$ (4).

References

1. Robinson, M. et al *Cancer Lett. (Shannon, Irel.)* 1989, **48**(3), 197-203.
2. Blazak, W. F. et al *Mutat. Res.* 1988, **206**(4), 431-438.
3. Meier, J. R. et al *Mutat. Res.* 1985, **157**, 111-122.
4. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T228 1,1,3-trichloroacetone



$\text{C}_3\text{H}_3\text{Cl}_3\text{O}$

Mol. Wt. 161.41

CAS Registry No. 921-03-9

Synonyms α,α',α' -trichloroacetone; 1,1,3-trichloro-2-propanone

EINECS No. 213-063-6

RTECS No. UC 3840000

Physical properties

M. Pt. 13-15°C B. Pt. 172°C Flash point 79°C Specific gravity 1.508

Mammalian & avian toxicity

Acute data

LC₅₀ (2 hr) inhalation mouse, rat 360-390 mg kg⁻¹ (1).

Carcinogenicity and chronic effects

Dermal mice (24 wk) 50 mg kg⁻¹ in ethanol 6 × over 2 wk. Two wk later animals received 1 μg 12-*o*-tetradecanoylphorbol-13-acetate topically 3 × wk⁻¹ for 20 wk. At the end of the study skin papillomas were seen in 4/39 mice (2).

Oral mice (24 wk) total dose of 150 kg⁻¹ then treated topically as above. Skin papillomas were seen in 3/34 mice (2).

Genotoxicity

Salmonella typhimurium positive (strains and metabolic activation unspecified) (3).
Saccharomyces cerevisiae D7 gene conversion with and without metabolic activation positive, XV185-14C reversion with metabolic activation weakly positive (3).

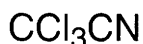
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level 1 $\mu\text{g l}^{-1}$ (4).

References

1. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
2. Robinson, M. et al *Cancer Lett. (Shannon, Irel.)* 1989, **48**(3), 197-203.
3. Nestmann, E. R. et al *Mutat. Res.* 1985, **155**, 53-60.
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T229 trichloroacetonitrile



$\text{C}_2\text{Cl}_3\text{N}$

Mol. Wt. 144.39

CAS Registry No. 545-06-2

Synonyms cyanotrichloromethane; 2,2,2-trichloroacetonitrile; trichloromethyl cyanide; trichloromethylnitrile; Tritox

EINECS No. 208-885-7

RTECS No. AM 2450000

Uses Organic synthesis. Insecticide.

Physical properties

M. Pt. -42°C **B. Pt.** $83-84^\circ\text{C}$ **Specific gravity** 1.4403 at 20°C with respect to water at 4°C

Volatility v.p. 58 mmHg at 20°C

Solubility Water: $<1\text{ g l}^{-1}$ at 21°C . Organic solvents: acetone, dimethyl sulfoxide, ethanol

Occupational exposure

Supply classification toxic

Risk phrases Toxic by inhalation, in contact with skin and if swallowed (R23/24/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S45)

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird $>100\text{ mg kg}^{-1}$ (1).

LD₅₀ oral rat 250 mg kg^{-1} (2).

LC_{Lo} (4-5 hr) inhalation rat, rabbit, guinea pig 250-310 ppm (2,3).

LD₅₀ dermal rabbit 900 mg kg^{-1} (2).

LD₅₀ intravenous mouse 56 mg kg^{-1} (4).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (5).

Gavage mouse (7 month) $10\text{ mg kg}^{-1} 3 \times \text{wk}^{-1}$ for 8 wk. Survival was not significantly different from controls.

Lung tumours developed in 9/32 treated animals compared with 3/31 controls (6).

Dermal mouse (1 yr) 0 or $80\text{ mg kg}^{-1} 3 \times \text{wk}^{-1}$ for 24 wk. No skin tumours occurred (7).

Dermal mouse tumour initiation-promotion study (1 yr) 0, 200, 400 or $800\text{ mg kg}^{-1} 3 \times \text{wk}^{-1}$ for 2 wk. 2 wk after the last application $1\text{ }\mu\text{g}$ 12-O-tetradecanoylphorbol-13-acetate animal⁻¹ was applied $3 \times \text{wk}^{-1}$ for 20 wk. A significant increase in skin papillomas and carcinomas was observed in the 400 mg kg^{-1} group compared with controls (7).

Teratogenicity and reproductive effects

Gavage rat 0, 1, 7.5, 15, 35 or $55\text{ mg kg}^{-1} \text{ day}^{-1}$ on days 6-18 of gestation. The high dose was lethal to 21% of the dams and induced 100% resorptions in 67% of the survivors. Foetal weight was reduced, and embryoletality was

observed in all treated groups in a dose-dependent manner. Cardiovascular and congenital malformations occurred in a dose-dependent manner (8).

Metabolism and toxicokinetics

Following gavage administration of 108 mg kg⁻¹ to rats, 2.3% of the dose was eliminated in the urine as thiocyanate within 24 hr. Metabolism involves formation of the corresponding cyanohydrin and the elimination of the cyanide, which is metabolised to thiocyanate by rhodanase (5,9).

Irritancy

Dermal rabbit (24 hr) 5 mg caused severe irritation and 50 µg instilled into rabbit eye for 24 hr caused severe irritation (10).

Genotoxicity

Salmonella typhimurium TA100, TA1535, TA1537 with and without metabolic activation positive (11).

In vitro Chinese hamster ovary cells sister chromatid exchanges positive (6).

In vitro human lymphoblasts DNA strand breaks positive (12,13).

In vivo rat liver γ-glutamyltranspeptidase-positive foci bioassay negative (14).

In vivo mouse bone marrow micronucleus test negative (6).

In vivo mouse sperm morphology assay negative (15).

Other effects

Any other adverse effects

Inhalation is very damaging to the upper respiratory tract and bronchi, and may be fatal. In animal studies, survivors suffered severe degenerative heart, liver and kidney lesions (16).

Death is preceded by ataxia and convulsions in rabbits (16).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (17).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (18).

WHO Guideline value for drinking water 1 µg l⁻¹ (provisional) (9).

Other comments

Disinfectant by-product in chlorinated drinking water (19,5).

Physical properties, uses, occurrence, carcinogenicity, mammalian toxicity and safety precautions reviewed (5,13).

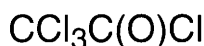
Reviews on human health effects, experimental toxicology, physico-chemical properties listed (20).

References

1. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
2. Smyth, H. et al *Am. Ind. Hyg. Assoc. J.* 1962, **23**, 95.
3. *J. Ind. Hyg. Toxicol.* 1949, **31**, 235.
4. Report NX 06416, US Army Armament Research and Development Command, Chemical Systems Laboratory, Aberdeen Proving Ground, MD 21010, USA.
5. IARC Monograph 1991, **52**, 269-296.
6. Bull, R. J. et al *Water Chlorination: Chemistry, Environmental Impact and Health Effects* 1985, Jolly, R. L. et al (Eds.) **5**, 21-227, Lewis Publishers, Chelsea, MI, USA.
7. Bull, R. J. et al *Fundam. Appl. Toxicol.* 1985, **5**, 1065-1074.
8. Smith, M. K. et al *Teratology* 1988, **38**(2), 113-120.
9. Piera, M. A. et al *J. Toxicol. Environ. Health* 1984, **13**, 633-641.
10. Marhold, J. V. *Prehled Prumyslove Toxikologie: Organické Latky* 1986, Prague, Czechoslovakia.
11. Mortelmans, K. et al *Environ. Mutagen.* 1986, **8**(Suppl. 7), 1-119.
12. Daniel, F. B. et al *Fundam. Appl. Toxicol.* 1986, **6**(3), 447-453.
13. *Chemical Safety Data Sheets* 1991, **4b**, 228-230, The Royal Society of Chemistry, London, UK.

14. Herren-Freund, S. L. et al *Environ. Health Perspect.* 1986, **69**, 59-65.
15. Meier, J. R. et al *Environ. Mutagen.* 1985, **7**, 201-211.
16. Gosselir, R. E. et al *Clinical Toxicology of Commercial Products* 5th ed., 1984, Williams and Wilkins, Baltimore, MD, USA.
17. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
18. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
19. *Guidelines for Drinking Water Quality* 2nd ed., 1991, **1**, WHO, Geneva, Switzerland.
20. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T230 trichloroacetyl chloride



$\text{C}_2\text{Cl}_4\text{O}$

Mol. Wt. 181.83

CAS Registry No. 76-02-8

Synonyms trichloroacetic acid chloride

EINECS No. 200-926-7

RTECS No. AO 7140000

Uses Organic synthesis. Derivatisation reagent in gas chromatography of sympathomimetic amines.

Physical properties

M. Pt. -146°C **B. Pt.** $114-116^\circ\text{C}$ **Specific gravity** 1.629 at 20°C with respect to water at 4°C

Volatility v.p. 16 mmHg at 20°C

Solubility Organic solvents: diethyl ether, ethanol

Occupational exposure

UN No. 2442 **HAZCHEM Code** 4X **Conveyance classification** corrosive substance

Mammalian & avian toxicity

Acute data

LD_{50} oral rat 600 mg kg^{-1} (1).

LC_{50} (4 hr) inhalation rat 475 mg m^{-3} (1).

Genotoxicity

Salmonella typhimurium TA98, TA100 with and without metabolic activation negative (2).

Other effects

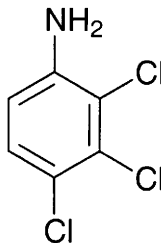
Other adverse effects (human)

Extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema (3).

References

1. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
2. Reichert, D. et al *Mutat. Res.* 1983, **117**(1-2), 21-30.
3. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3406, Sigma-Aldrich, Milwaukee, WI, USA

T231 2,3,4-trichloroaniline



$C_6H_4Cl_3N$

Mol. Wt. 196.46

CAS Registry No. 634-67-3

Synonyms 2,3,4-trichlorobenzenamine

EINECS No. 211-215-6

Physical properties

M. Pt. 65-67°C B. Pt. 292°C at 774 mmHg Partition coefficient $\log P_{ow}$ 3.17 (1)

Solubility Organic solvents: ethanol, ligroin

Occupational exposure

Supply classification toxic

Risk phrases Toxic by inhalation, in contact with skin and if swallowed – Danger of cumulative effects (R23/24/25, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – After contact with skin, wash immediately with plenty of water – Wear suitable protective clothing and gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S28, S36/37, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (14 day) guppy 1.3 mg l⁻¹ (1).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 2.4 ppm Microtox test (2).

Bioaccumulation

Bioconcentration factor in guppy 800-2000 (3).

Mammalian & avian toxicity

Irritancy

Irritating to the skin, eyes, mucous membranes and upper respiratory tract (species unspecified) (4).

Genotoxicity

Salmonella typhimurium TA98, TA100 with and without metabolic activation negative (5).

Other effects

Other adverse effects (human)

Absorption into the body leads to the formation of methaemoglobin, which in sufficient concentration causes cyanosis (4).

Any other adverse effects

Intraperitoneal rat, single dose of 150 or 300 mg kg⁻¹ did not affect renal function markedly. However, *in vitro* 200 mg l⁻¹ was effective in decreasing tetraethylammonium and *p*-aminohippurate accumulation by renal cortical slices (6).

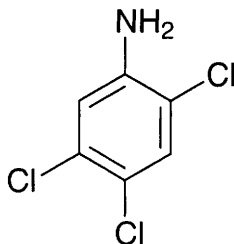
Legislation

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (7).

References

1. Leegwater, D. C. *Aquat. Toxicol.* 1989, **15**(2), 157-168.
2. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
3. De Wolf, W. et al *Comp. Biochem. Physiol.* 1991, **100C**(1-2), 55-57.
4. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3406, Sigma-Aldrich, Milwaukee, WI, USA.
5. Rashid, K. A. et al *J. Environ. Sci. Health, Part B* 1987, **B22**(6), 721-729.
6. Lo, H. H. et al *Toxicol. Lett.* 1991, **57**(3), 319-328.
7. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK

T232 2,4,5-trichloroaniline



C₆H₄Cl₃N

Mol. Wt. 196.46

CAS Registry No. 636-30-6

Synonyms 2,4,5-trichlorobenzenamine

EINECS No. 211-254-9

Physical properties

M. Pt. 93-95°C B. Pt. 270°C Partition coefficient log P_{ow} 3.17 (1)

Solubility Organic solvents: carbon disulfide, diethyl ether, ethanol, ligroin

Occupational exposure

Supply classification toxic

Risk phrases Toxic by inhalation, in contact with skin and if swallowed – Danger of cumulative effects (R23/24/25, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – After contact with skin, wash immediately with plenty of water – Wear suitable protective clothing and gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S28, S36/37, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (14 day) guppy 1.9 mg l⁻¹ (1).

LC₅₀ (28 day) zebra fish 0.12 mg l⁻¹ (2).

Invertebrate toxicity

LC₅₀ (30 min) *Photobacterium phosphoreum* 1.5 ppm Microtox test (3).

Bioaccumulation

Bioconcentration factor for guppy 1300-2500 (4).

Mammalian & avian toxicity

Irritancy

Irritating to the eyes, skin, mucous membranes and upper respiratory tract (species unspecified) (5).

Genotoxicity

In vitro primary rat hepatocytes DNA repair assay negative (6).

Other effects

Other adverse effects (human)

Absorption into the body leads to the formation of methaemoglobin, which in sufficient concentration causes cyanosis (5).

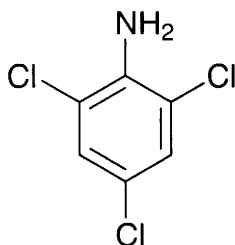
Legislation

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (7).

References

1. Leegwater, D. C. *Aquat. Toxicol.* 1989, **15**(2), 157-168.
2. Van Leewuen, C. J. et al *Aquat. Toxicol.* 1990, **16**(4), 321-334.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. De Wolf, W. et al *Comp. Biochem. Physiol.* 1991, **100C**, (1-2), 55-57.
5. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3407, Sigma-Aldrich, Milwaukee, WI, USA.
6. Yoshimi, N. et al *Mutat. Res.* 1988, **206**(2), 183-191.
7. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK

T233 2,4,6-trichloroaniline



$C_6H_4Cl_3N$

Mol. Wt. 196.46

CAS Registry No. 634-93-5

Synonyms *sym*-trichloroaniline; 2,4,6-trichlorobenzeneamine

EINECS No. 211-219-8

RTECS No. BZ 0250000

Uses In photographic materials.

Physical properties

M. Pt. 73-75°C **B. Pt.** 262°C **Partition coefficient** $\log P_{ow}$ 3.52 (1)

Solubility Organic solvents: carbon disulfide, diethyl ether, ethanol, light petroleum

Occupational exposure

Supply classification toxic

Risk phrases Toxic by inhalation, in contact with skin and if swallowed – Danger of cumulative effects (R23/24/25, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – After contact with skin, wash immediately with plenty of water – Wear suitable protective clothing and gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S28, S36/37, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow 1-10 mg l⁻¹ (2).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 4.6 ppm Microtox test (3).

Bioaccumulation

Bioconcentration factor for guppy 3200 (4).

Environmental fate

Degradation studies

Biodegradation by *Aerobacter* sp. 500 mg l⁻¹ at 30°C: 82% ring disruption by parent strains in 120 hr; 100% by mutant strains in 30 hr (5).

Abiotic removal

Degraded by sunlight and rapidly evaporates from water (6).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 1200-3850, 5800 mg kg⁻¹, respectively (7,8).

LD₅₀ intraperitoneal rat, mouse 800 mg kg⁻¹ (9).

Intraperitoneal rat, single dose of 150 or 300 mg kg⁻¹ did not affect renal function markedly (10).

Carcinogenicity and chronic effects

Oral rat, mouse (18 month) 3000-12,000 mg kg⁻¹ diet produced a significant increase in vascular tumours in ♂ mice. An increase in hepatocellular carcinomas was also reported (11).

Irritancy

Irritating to the skin, eyes, mucous membranes and upper respiratory tract (species unspecified) (12).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535 with and without metabolic activation negative (13,14).

Drosophila melanogaster wing spot test positive (15).

In vitro primary rat hepatocytes DNA repair assay negative (16).

Other effects

Other adverse effects (human)

Absorption into the body leads to the formation of methaemoglobin which in sufficient concentration causes cyanosis (12).

Legislation

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (17).

Other comments

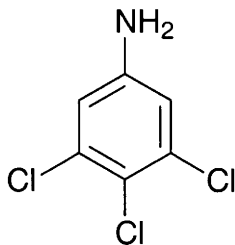
Residues have been isolated from natural waters (18).

Physical properties, uses, toxicity and safety precautions reviewed (19).

References

1. Camilleri, P. et al *J. Chem. Soc. Perkin Trans. II* 1988, 1699-1707.
2. US EPA WPC Research Series 12020 EXG 1972.
3. Kaiser, K. L. E. et al et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. De Wolf, W. et al *Comp. Biochem. Physiol.* 1991, **100C**(1-2), 55-57.
5. Worne, H. E. *Tijdschrift van Let BECEWA* Liege, Belgium.
6. Dennis, W. H. et al *Ins. Unsambrdl.-TR.8202* 1983, Order No. AD-A133937 (*Chem. Abstr.* **100**, 152413h).
7. *Gig. Sanit.* 1985, **30**, 83.
8. *Gig. Sanit.* 1990, **55**(6), 86.
9. *Report OTS 206512* US EPA Office of Toxic Substances.
10. Lo, H. H. et al *Toxicol. Lett.* 1991, **57**(3), 319-328.
11. Wesiburger, E. K. et al *J. Environ. Pathol. Toxicol.* 1978, **2**, 325.
12. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3407, Sigma-Aldrich, Milwaukee, WI, USA.
13. Zeiger, E. et al *Environ. Mol. Mutagen.* 1992, **19**(Suppl. 21), 2-141.
14. Zimmer, D. et al *Mutat. Res.* 1980, **77**, 319.
15. Kugler-Steigmeir, M. E. et al *Mutat. Res.* 1989, **211**(2), 279-289.
16. Yoshimi, N. et al *Mutat. Res.* 1988, **206**(2), 183-191.
17. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
18. Richardson, M. L. *Compendium of Toxicological Ecological Data on Chemicals Found by GC-MS in Water Samples* 1985, Thames Water, Reading, UK.
19. *Chemical Safety Data Sheets* 1991, **4b**, 231-233, The Royal Society of Chemistry, London, UK

T234 3,4,5-trichloroaniline



$C_6H_4Cl_3N$

Mol. Wt. 196.46

CAS Registry No. 634-91-3

Synonyms 3,4,5-trichlorobenzenamine

EINECS No. 211-218-2

Uses Organic synthesis.

Physical properties

M. Pt. 98-100°C Partition coefficient $\log P_{ow}$ 3.58 (1)

Solubility Organic solvents: ethanol

Occupational exposure

UN No. 2811

Supply classification toxic

Risk phrases Toxic by inhalation, in contact with skin and if swallowed – Danger of cumulative effects (R23/24/25, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – After contact with skin, wash immediately with plenty of water – Wear suitable protective clothing and gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S28, S36/37, S45)

Ecotoxicity

Fish toxicity

Fatal to stickleback in 4-6 hr and to brown trout in 8-12 hr at 30 mg l⁻¹ (2).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 3.3 ppm Microtox test (3).

Bioaccumulation

Bioaccumulation factor for guppy 2100-4000 (4).

Mammalian & avian toxicity

Acute data

Intraperitoneal rat, single dose of 150 or 300 mg kg⁻¹ did not affect renal function significantly (5).

Irritancy

Irritating to the skin, eyes, mucous membranes and upper respiratory tract (species unspecified) (6).

Genotoxicity

Salmonella typhimurium TA98, TA100 with and without metabolic activation negative (7).

Other effects

Other adverse effects (human)

Absorption into the body leads to the formation of methaemoglobin, which in sufficient concentration causes cyanosis (6).

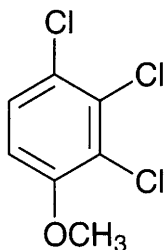
Legislation

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (8).

References

1. Camilleri, P. et al *J. Chem. Soc. Perkin Trans. II* 1988, 1699-1707.
2. McPhee, C. et al *Lethal Effects of 2014 Chemicals to Fish* 1989, EPA 560/6-89-001; PB 89-156-715, Washington, DC, USA.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. De Wolf, W. et al *Comp. Biochem. Physiol.* 1991, **100C**(1-2), 55-57.
5. Lo, H. H. et al *Toxicol. Lett.* 1991, **57**(3), 319-328.
6. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3408.
7. Rashid, K. A. et al *J. Environ. Sci. Health, Part B* 1987, **B22**(6), 721-729.
8. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK

T235 2,3,4-trichloroanisole



$C_7H_5Cl_3O$

Mol. Wt. 211.47

CAS Registry No. 54135-80-7

Synonyms 1,2,3-trichloro-4-methoxybenzene

EINECS No. 258-990-7

Physical properties

M. Pt. 69-71°C

Ecotoxicity

Invertebrate toxicity

EC₅₀ (48 hr) *Minutocellus polymorphus* 0.40 mg l⁻¹ (1).

EC₅₀ (72 hr) *Skeletonema costatum* 0.63 mg l⁻¹ (1).

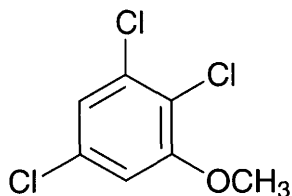
Bioaccumulation

Guppies kept in a tank containing 2462 µg for 7 days had 71 µg in their tissues (2).

References

1. Walsh, G. E. et al *Environ. Toxicol. Chem.* 1988, 7(11), 925-929.
2. Opperhuizen, A. et al *Chemosphere* 1987, 16(5), 953-962

T236 2,3,5-trichloroanisole



$C_7H_5Cl_3O$

Mol. Wt. 211.47

CAS Registry No. 54135-81-8

Synonyms 1,2,5-trichloro-3-methoxybenzene

Physical properties

M. Pt. 84°C

Ecotoxicity

Invertebrate toxicity

≤790 µg ml⁻¹ did not inhibit growth of 18 bacterial species (1).

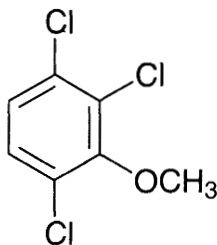
Bioaccumulation

Guppies kept in tank containing 1526 µg for 7 days had 35 µg in their tissues (2).

References

1. Ruckdeschel, G. et al *Appl. Environ. Microbiol.* 1987, 53(11), 2689-2692.
2. Opperhuizen, A. et al *Chemosphere* 1987, 16(5), 953-962

T237 2,3,6-trichloroanisole



$C_7H_5Cl_3O$

Mol. Wt. 211.47

CAS Registry No. 50375-10-5

Synonyms 1,2,4-trichloro-3-methoxybenzene

Physical properties

M. Pt. 40-45°C B. Pt. 227-229°C at 756 mmHg

Solubility Organic solvents: ethyl alcohol

Ecotoxicity

Invertebrate toxicity

LC₅₀ (48 hr) *Minutocellus polymorphus* 0.82 mg l⁻¹ (1).

EC₅₀ (72 hr) *Skeletonema costatum* 0.56 mg l⁻¹ (1).

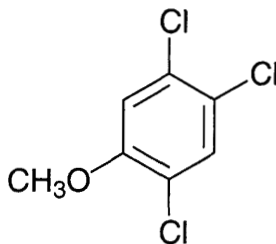
Bioaccumulation

Guppies kept for 7 day in a tank containing 450 µg had 2 µg in their tissues (2).

References

1. Walsh, G. E. et al *Environ. Toxicol. Chem.* 1988, 7(11), 925-929.
2. Opperhuizen, A. et al *Chemosphere* 1987, 16(5), 953-962

T238 2,4,5-trichloroanisole



$C_7H_5Cl_3O$

Mol. Wt. 211.47

CAS Registry No. 6130-75-2

Synonyms 1,2,4-trichloro-5-methoxybenzene

EINECS No. 228-099-8

Ecotoxicity

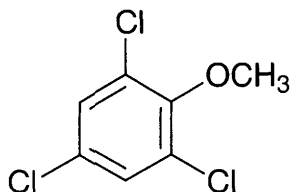
Bioaccumulation

Guppies kept in a tank containing 1170 µg for 7 days had 22 µg (estimated) in their tissues (1).

References

1. Opperhuizen, A. et al *Chemosphere* 1987, 16, (5), 953-962

T239 2,4,6-trichloroanisole



C₇H₅Cl₃O

Mol. Wt. 211.47

CAS Registry No. 87-40-1

Synonyms 1,3,5-trichloro-2-methoxybenzene; methyl 2,4,6-trichlorophenyl ether; Tyrene

EINECS No. 201-743-5

Uses Formerly used as a dye adjunct for polyester fibres.

Physical properties

M. Pt. 60°C **B. Pt.** 240°C at 738.2 mmHg

Solubility Organic solvents: benzene, cyclohexanone, dioxane, methanol

Ecotoxicity

Invertebrate toxicity

EC₅₀ (48 hr) *Minutocellus polymorphus* 0.03 mg l⁻¹ (1).

EC₅₀ (72 hr) *Skeletonema costatum* 0.63 mg l⁻¹ (1).

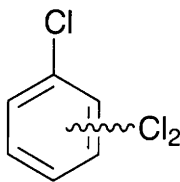
Bioaccumulation

Guppies kept in water containing 350 µg were estimated to have 2 µg in their tissues after 7 days (2).

References

1. Walsh, G. E. et al *Environ. Toxicol. Chem.* 1988, 7(11), 925-929.
2. Opperhuizen, A. et al *Chemosphere* 1987, 16(5), 953-962

T240 trichlorobenzene (technical mixture)



$C_6H_3Cl_3$

Mol. Wt. 181.45

CAS Registry No. 12002-48-1

EINECS No. 234-413-4

Uses Solvent.

Physical properties

B. Pt. 205-250°C Volatility v.den. 1.460

Solubility Organic solvents: benzene, carbon disulfide, ethanol

Occupational exposure

DE-MAK 5 ppm (38 mg m⁻³)

UN No. 2321 HAZCHEM Code Z2 Conveyance classification toxic substance

Environmental fate

Degradation studies

Degraded by aerobic bacterial culture isolated from soil, with the incorporation of carbon from the substrate into cell biomass and conversion into carbon dioxide (1).

Degraded by *Pseudomonas*, *Alcaligenes* and *Moraxella* species isolated from the River Rhine and from industrial wastewater treatment plants (2).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (3).

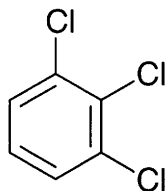
Tolerable daily intake (TDI) human 7.7 µg kg⁻¹ (4).

WHO guideline value for drinking water 20 µg l⁻¹ (4).

References

1. Swindoll, C. M. et al *Environ. Toxicol. Chem.* 1988, 7(4), 291-299.
2. Springer, W. et al *Gas-Wasserfach: Wasser/Abwasser* 1988, 129(1), 70-75 (Ger.) (*Chem. Abstr.* 108, 164514v).
3. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
4. *Guidelines for Drinking Water Quality* 2nd ed., 1993, 1, WHO, Geneva, Switzerland

T241 1,2,3-trichlorobenzene



$C_6H_3Cl_3$

Mol. Wt. 181.45

CAS Registry No. 87-61-6

Synonyms *vic*-trichlorobenzene

EINECS No. 201-757-1

RTECS No. DC 2095000

Uses Solvent for high melting point products. Coolant in electrical installations. Organic synthesis. A commercial grade (mixture of isomers) is used to combat termites.

Physical properties

M. Pt. 53-55°C B. Pt. 218-219°C Flash point 126°C Specific gravity 1.69 at 25°C with respect to water at 25°C Partition coefficient $\log P_{ow}$ 4.20 (1) Volatility v.p. 1 mmHg at 40°C; v.den. 6.26
Solubility Water: insoluble in water. Organic solvents: benzene, carbon disulfide, ethanol

Occupational exposure

DE-MAK 5 ppm (38 mg m⁻³)

UN No. 2321 HAZCHEM Code ZZ Conveyance classification toxic substance

Ecotoxicity

Fish toxicity

LC₅₀ (14 day) guppy 2.4 ppm (2).

LC₅₀ (28 day) zebra fish 0.99 mg l⁻¹ (3).

LD₅₀ intraperitoneal rainbow trout 1600 mg kg⁻¹ (4).

Mosquito fish (*Gambusia affinis*) exposed for 42 days to sublethal concentrations of 1,2,3-trichlorobenzene as low as 0.18 µmol l⁻¹ suffered growth rate reduction. EC₅₀ and EC₁₀ values for four halobenzenes (1,4-dibromobenzene, 1,2,3-trichlorobenzene, 1,2,4-tribromobenzene, and pentachlorobenzene) were 0.067-3.4 and 0.00042-0.32 µmol, respectively (within the ranges 5 to 8% and 0.1 to 3.9% of the LC₅₀ values) (5).

Invertebrate toxicity

EC₅₀ (48 hr) *Daphnia magna* 2.8 mg l⁻¹ (1).

EC₅₀ (30 min) *Photobacterium phosphoreum* 3.2 ppm Microtox test (6).

Bioaccumulation

Bioconcentration factor for guppy 13,000 (on lipid content) and ~200 for the bacterium *Siderocapsa* sp. (2).

Environmental fate

Nitrification inhibition

IC₅₀ (25 day) *Nitrosomonas* sp. 96 mg l⁻¹ (7).

Anaerobic effects

IC₅₀ (50 day) methanogenic bacterial culture 24 mg l⁻¹ (7).

Degradation studies

Partially degraded when incubated anaerobically with sewage sludge for 32 days (8).

Sparingly degraded when incubated with natural river water, spring water and sea water (9).

Degradation by *Pseudomonas* sp. (200 mg l⁻¹ and 30°C); parent strains 87% ring disruption in 120 hr, mutant strains 100% ring disruption in 43 hr (10).

Adsorption and retention

K_{oc} in clay loam, sandy loam, and light clay soils 1500-2700 (11).

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal mouse 1400 mg kg⁻¹ (12).

Sub-acute and sub-chronic data

Oral rat 1, 10, 100 or 1000 ppm in diet for 13 wk. High-dose ♂ rats had reduced weight gain and relative increased liver and kidney weights. Moderate histological changes were observed in the liver and thyroid in ♂ rats (13).

Teratogenicity and reproductive effects

Gavage rat 150, 300 or 600 mg kg⁻¹ day⁻¹ on days 6-15 of gestation causes no teratogenic or foetotoxic effects. No accumulation was observed in maternal or foetal tissues. Of the 3 isomers tested 1,2,4-trichlorobenzene exhibited the highest maternal toxicity (14).

Metabolism and toxicokinetics

Following oral administration of 10 mg kg⁻¹ radio-labelled compound to fasted rats, radioactivity appeared in the blood and tissues within 30 min and peaked 2-4 hr after dosing. Fat, skin and liver contained high concentrations of parent compound, while the kidneys and muscle had high concentrations of metabolites. 95% of the dose was eliminated within 48 hr in the urine and faeces, with the former being the major route (15).

Irritancy

Irritating to the skin, eyes and upper respiratory tract (species unspecified) (16).

Genotoxicity

Salmonella typhimurium TA100 with and without metabolic activation negative (17).

In vivo rat liver foci bioassay positive (18).

In vivo mouse bone marrow micronucleus test positive (12,19).

Legislation

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (20).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (21).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (22).

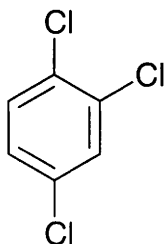
Residues have been detected in fish tissues and water samples (23-25).

References

1. Vighi, M. et al *Chemosphere* 1987, **16**(5), 1043-1051.
2. Konemann, W. H. *Quantitative Structure-Activity Relationships for Kinetics and Toxicity of Aquatic Pollutants and Their Mixtures in Fish* 1979, Univ. Utrecht, Netherlands.
3. van Leeuwen, C. J. et al *Aquat. Toxicol.* 1990, **16**(4), 321-334.
4. Hodson, P. V. et al *Environ. Toxicol. Chem.* 1988, **7**(6), 443-454.
5. Chaisuksant, Y. et al *Ecotoxicol. Environ. Saf.* 1998, **39**(2), 120-130.
6. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
7. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, **63**(3), 198-207.
8. Kirk, P. W. W. et al *Chemosphere* 1989, **18**(9-10), 1771-1784.
9. Niinomi, J. et al *Mie-Ken Kerkyo Kagaku Senta Kerkyo Hokoku* 1989, (9), 53-60 (Japan.) (*Chem. Abstr.* **111**, 189142x).
10. Worne, H. E. *Tijdschrift van Let BECEWA* Liege, Belgium.
11. Kishi, H. et al *Chemosphere* 1990, **21**(7), 867-876.

12. Mohtashamipur, E. et al *Mutagenesis* 1987, **2**(2), 111-117.
13. Cote, M. et al *Drug Chem. Toxicol.* 1988, **11**(1), 11-28.
14. Rupa, D. S. et al *Bull. Environ. Contam. Toxicol.* 1988, **41**(5), 737-741.
15. Chu, I. et al *J. Environ. Sci. Health, Part B* 1987, **B22**(4), 439-453.
16. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3409, Sigma-Aldrich, Milwaukee, WI, USA.
17. Klopman, G. et al *Mol. Toxicol.* 1987, **1**, 61-81.
18. Hermen-Freund, S. L. et al *Environ. Health Perspect.* 1986, **69**, 59-65.
19. Parrini, M. et al *Boll.-Soc. Ital. Biol. Sper.* 1990, **66**(7), 709-716.
20. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
21. S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations 1991, HMSO, London, UK.
22. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium.
23. Verschuere, K. *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, 1122, Van Nostrand Reinhold, New York, NY, USA.
24. Rogers, H. R. et al *Mar. Pollut. Bull.* 1989, **20**(6), 276-281.
25. Ofstad, E. B. et al *Sci. Total Environ.* 1978, **10**, 219-230

T242 1,2,4-trichlorobenzene



$C_6H_3Cl_3$

Mol. Wt. 181.45

CAS Registry No. 120-82-1

Synonyms *unsym*-trichlorobenzene

EINECS No. 204-428-0

RTECS No. DC 2100000

Uses Solvent. Dielectric fluid. Organic synthesis.

Physical properties

M. Pt. 16°C B. Pt. 214°C Flash point >110°C Specific gravity 1.454 at 25°C with respect to water at 25°C

Partition coefficient $\log P_{ow}$ 4.02 (1) Volatility v.p. 1 mmHg at 28.4°C; v.den. 6.26

Solubility Water: 49 mg l⁻¹ at 20°C. Organic solvents: benzene, carbon disulfide, diethyl ether, ethanol, light petroleum, isopropanol

Occupational exposure

UK-LTEL 5 ppm (38 mg m⁻³)

UK-STEL 5 ppm (38 mg m⁻³)

US-STEL ceiling limit 5 ppm

UN No. 2321 HAZCHEM Code Z2 Conveyance classification toxic substance

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow 30.0 mg l⁻¹ flow-through bioassay (2).

LC₅₀ (14 day) guppy 2.4 ppm (3).
LD₅₀ intraperitoneal rainbow trout 1800 mg kg⁻¹ (4).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 4.0 ppm Microtox test (5).

Bioaccumulation

Bioconcentration factors for fathead minnow, rainbow trout, golden ide, bluegill sunfish ranged between 490-5200 (6-9).

Bioconcentration factor 51 for rainbow trout muscle (8 hr static bioassay); bioconcentration factor 89 (35 day flow-through bioassay) (10).

A first-order one-compartment model gave uptake and elimination rate constants of 492 ± 234 l kg⁻¹ day⁻¹ and 0.49 ± 0.22 day⁻¹, respectively, for guppies exposed to sublethal concentrations of 1,2,4-trichlorobenzene (11).

Environmental fate

Nitrification inhibition

IC₅₀ (25 day) *Nitrosomonas* sp. 210 mg l⁻¹ (2).

Carbonaceous inhibition

IC₅₀ (5 day) aerobic heterotrophs isolated from activated sludge 7700 mg l⁻¹ (2).

Anaerobic effects

IC₅₀ (50 day) methanogenic bacterial culture 120 mg l⁻¹ (2).

Degradation studies

Degraded by *Pseudomonas* sp., initially forming dihydrates which undergo dearomatisation to yield 3,4,6-trichlorocatechol, and subsequently *ortho*-cleavage to form 2,3,5-trichloro-*cis,cis*-muconate (12).

Partially degraded when incubated with sewage sludge for 32 days (13).

Abiotic removal

Exposure of 20 g to sunlight for 56 days led to formation of 1% polychlorinated biphenyl (14).

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated $t_{1/2}$ 18.5 days (15).

Evaporation from model river water, estimated $t_{1/2}$ 4.2 hr (16).

Evaporation from seawater model 11-22 days (17).

Adsorption and retention

Reported K_{oc} 1000-5000 (18-20).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 300, 750 mg kg⁻¹, respectively (21,22).

LD₅₀ intraperitoneal mouse 1200 mg kg⁻¹ (23).

Sub-acute and sub-chronic data

Oral rat 1, 10, 100 or 1000 ppm in diet for 13 wk. Increased liver and kidney weights were observed in high dose ♂ rats. An increase in hepatic aminopyrine demethylase and aniline hydroxylase activities in ♂, and aminopyrine demethylase activity in ♀ was observed in the high-dose group. Moderate histological changes were seen in the liver and thyroid of high-dose ♂ rats (24).

Inhalation rat, no-adverse-effect level 20 ppm 6 hr day⁻¹ for 15 days (25).

Teratogenicity and reproductive effects

Gavage rat 75, 150 or 300 mg kg⁻¹ day⁻¹ on days 6-15 of gestation caused no teratogenic or foetotoxic effects. No accumulation was observed in maternal or foetal tissues. Of the 3 isomers tested, 1,2,4-trichlorobenzene exhibited the highest maternal toxicity (26).

Oral rat (day 9-13 of gestation) 0, 36, 120, 360, 1200 mg kg⁻¹ day⁻¹. Maternal deaths were recorded in 2/9 rats given 360 mg kg⁻¹ and 6/6 given 1200 mg kg⁻¹. Embryo lethality and embryonic development (parameters tested were head length, crown-rump length, somite number and protein content) were significantly retarded (27).

Rats were continuously exposed to 0, 25, 100 or 400 ppm in drinking water for 3 generations (F₀ to F₂). The treatment did not affect fertility, growth, viability, locomotor activity or blood chemistry. Adrenal enlargement was observed in both F₀ and F₁ generations (28).

Metabolism and toxicokinetics

Metabolised by rat liver microsomes *in vitro* to 2,3,6- and 2,4,5-trichlorophenol, and to a lesser extent 2,4,6- and 2,3,5-trichlorophenol and trichlorohydroquinone. ~10% of all metabolites became covalently bound to protein (29).

Following intragastric administration to rats, 1,2,4-trichlorobenzene was detected in all organs and tissues within 4 min. Most was found in the gastro-intestinal tract. After 24 hr ~20% was found in the gastro-intestinal tract, 6% in adipose tissue and ~2% in muscle. No accumulation was observed after repeated intragastric administration (30).

Following oral administration of 10 mg kg⁻¹ to fasted rats, radioactivity appeared in the blood and tissues within 0.5 hr and peaked at 2-4 hr after dosing. Fat, skin and liver contained high concentrations of parent compound while the kidneys and muscle had high levels of metabolites. Terminal t_{1/2} was 93 hr (31).

Irritancy

Dermal rabbit, 2000 mg applied intermittently over 13 wk caused moderate irritation (32).

Vapour or mist is irritating to the mucous membranes and upper respiratory tract (species unspecified) (33).

Genotoxicity

Salmonella typhimurium TA100 with and without metabolic activation negative (34).

In vivo rat liver foci bioassay positive (35).

In vivo mouse bone marrow micronucleus test positive (23,36).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (37).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (38).

Maximum admissible concentrations in drinking water (Russia) 0.03 mg l⁻¹ (39).

Other comments

Residues have been isolated from drinking water, natural waters, sediments, fish tissue and urban air samples (40).

Environmental fate reviewed (40).

Toxicity and health effects reviewed (41).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (42).

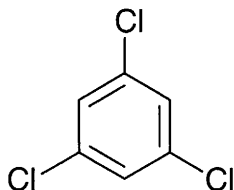
Autoignition temperature 571°C.

References

1. Hansch, C. et al *Medchem. Project Issue No. 26* 1985, Claremont College, Pomona, CA, USA.
2. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, 6(3), 198-207.
3. Konemann, W. H. *Quantitative Structure-Activity Relationships for Kinetics and Toxicity of Aquatic Pollutants and their Mixtures in Fish* 1979, Univ. Utrecht, Germany.
4. Hodson, P. V. et al *Environ. Toxicol. Chem.* 1988, 7(6), 443-454.
5. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, 26(3), 361-431.
6. Veith, G. D. et al *J. Fish Res. Board Can.* 1979, 36, 1040-1048.
7. Oliver, B. G. et al *Environ. Sci. Technol.* 1985, 19, 842-848.
8. Barrows, M. E. et al in *Dyn. Exposure Hazard Assess. Toxic. Chem.* 1980, 379-392, Ann Arbor Sci., MI, USA.
9. Freitag, D. et al *Chemosphere* 1985, 14, 1589-1616.
10. Spehar, R. L. et al *Environ. Toxicol. Chem.* 1985, 4, 131-142.
11. van Eck, J. M. C. et al *Chemosphere* 1997, 34(11), 2259-2270.
12. Sander, P. et al *DECHEMA Biotechnol. Conf.* 1990, 4(Pt A), 617-621.
13. Kirk, P. W. W. et al *Chemosphere* 1989, 18(9-10), 177, 1-1784.

14. Uyeta, M. et al *Nature* 1976, **264**, 583-584.
15. Atkinson, R. et al *Environ. Sci. Technol.* 1985, **19**, 87-89.
16. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behaviour of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
17. Wakeham, S. G. et al *Environ. Sci. Technol.* 1983, **17**, 611-617.
18. Wilson, J. T. et al *J. Environ. Qual.* 1981, **10**, 501-506.
19. Friesal, P. et al *Fresenius Z. Anal. Chem.* 1984, **319**, 160-164.
20. Chiou, P. E. et al *Environ. Sci. Technol.* 1983, **17**, 227-231.
21. *Nara Igaku Zasshi* 1978, **29**, 569.
22. *Annal. Occup. Hyg.* 1969, **12**, 209.
23. Mohtashamipur, E. et al *Mutagenesis* 1987, **2**(2), 111-117.
24. Cote, M. et al *Drug Chem. Toxicol.* 1988, **11**(1), 11-28.
25. *Material Safety Data Sheet* Dow Chemical Co., 1978.
26. Rupa, D. S. et al *Bull. Environ. Contam. Toxicol.* 1988, **41**(5), 737-741.
27. *Environ. Res.* 1983, **31**, 362.
28. *J. Toxicol. Environ. Health* 1981, **8**, 489.
29. Den Besten, P. J. et al *Toxicol. Appl. Pharmacol.* 1991, **108**(2), 223-233.
30. Khalturin, G. V. et al *Gig. Sanit.* 1988, (2), 86-87 (Russ.) (*Chem. Abstr.* **108**, 145026w).
31. Chu, I. et al *J. Environ. Sci. Health, Part B* 1987, **B22**(4), 439-453.
32. *Arch. Environ. Health* 1975, **30**, 165.
33. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3409, Sigma-Aldrich, Milwaukee, WI, USA.
34. Klopman, G. *Mol. Toxicol.* 1987, **17**, 61-81.
35. Hermen-Freund, S. L. et al *Environ. Health Perspect.* 1986, **69**, 59-65.
36. Parrini, M. et al *Boll.-Soc. Ital. Biol. Sper.* 1990, **66**(7), 709-716.
37. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
38. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; *6th Amendment EEC Directive* 79/831/EEC; *7th Amendment EEC Directive* 91/32/EEC 1991, HMSO, London, UK.
39. Bospamyatonov, G. P. et al *Maximum Allowable Concentrations of Environmental Chemicals* 1985, Khimiya, Leningrad, USSR.
40. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1989, **1**, 518-527, Lewis Publishers, Chelsea, MI, USA.
41. *US EPA Report* 1987, EPA/600/8-88/057, Washington, DC, USA.
42. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T243 1,3,5-trichlorobenzene



$C_6H_3Cl_3$

Mol. Wt. 181.45

CAS Registry No. 108-70-3

Synonyms *sym*-trichlorobenzene; TCB; TCBA

EINECS No. 203-608-6

RTECS No. DC 2100100

Uses Organic synthesis.

Physical properties

M. Pt. 63-65°C **B. Pt.** 208°C **Flash point** 126°C **Partition coefficient** $\log P_{ow}$ 4.49 (1) **Volatility** v.p. 0.578 mmHg at 25°C; v.den. 6.26
Solubility Water: 5.8 mg l⁻¹ at 20°C. Organic solvents: benzene, carbon disulfide, diethyl ether, ethanol, glacial acetic acid, light petroleum, ligroin

Occupational exposure

DE-MAK 5 ppm (38 mg m⁻³)

UN No. 2321 **HAZCHEM Code** 2Z **Conveyance classification** toxic substance

Ecotoxicity

Fish toxicity

LC₅₀ (14 day) guppy 3.3 mg l⁻¹ (2).

LD₅₀ intraperitoneal rainbow trout 5600 mg kg⁻¹ (3).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 14 ppm Microtox test (4).

Bioaccumulation

Bioaccumulation in guppy 14,000 (on lipid content) and ~250 in the bacterium *Siderocapsa treubii* (2).

Environmental fate

Nitrification inhibition

IC₅₀ (25 day) *Nitrosomonas* sp. 96 mg l⁻¹ (5).

Anaerobic effects

IC₅₀ (50 day) methanogenic bacterial culture 750 mg l⁻¹ (5).

Degradation studies

Sparingly degraded when incubated with natural river water, spring water and seawater (6).

25% degradation when incubated anaerobically with sewage sludge for 32 days (7).

Degradation by *Pseudomonas* sp. 200 mg l⁻¹ at 30°C, 78% disruption 120 hr by parent strains. 100% ring disruption in 50 hr by mutant strains (8).

Abiotic removal

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated t_{1/2} 6.17 months (9).

Exposure of 20 g to sunlight for 56 days led to the formation of 160 ppm polychlorinated biphenyls (10).

Adsorption and retention

Reported K_{oc} 1800 and 126,000 (11,12).

Estimated K_{oc} 6600 indicates that adsorption to soil and sediment would be significant (13).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 800, 350 mg kg⁻¹, respectively (14,15).

LD₅₀ intraperitoneal mouse 2300 mg kg⁻¹ (16).

Sub-acute and sub-chronic data

Oral rat 1, 10, 100 or 1000 ppm diet for 13 wk caused increased liver and kidney weights and moderate histological changes to the liver and thyroid in high-dose ♂ rats (17).

Teratogenicity and reproductive effects

Gavage rat 150, 300 or 600 mg kg⁻¹ day⁻¹ on days 6-15 of gestation. No teratogenic or foetotoxic effects were observed. Low levels of 1,3,5-trichlorobenzene accumulated in maternal adipose tissue, but not in foetal tissues. Of the 3 isomers tested, 1,2,4-trichlorobenzene exhibited the highest maternal toxicity (18).

Metabolism and toxicokinetics

Following oral administration of 10 mg kg⁻¹ ¹⁴C-labelled compound to fasted rats, radioactivity appeared in the blood and tissues within 30 min and peaked at 2-4 hr after dosing. Fat, skin and liver contained high concentrations of parent compound, while the kidneys and muscle had high concentrations of metabolites, 89% of the dose was eliminated within 48 hr in the urine and faeces, with the former being the major route (19).

Irritancy

Irritating to the skin, eyes, mucous membranes and upper respiratory tract (species unspecified) (20).

Genotoxicity

Salmonella typhimurium TA100 with and without metabolic activation negative (21).

In vivo rat liver foci bioassay positive (22).

In vivo mouse bone marrow micronucleus test positive (16,23).

Legislation

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (24).

Other comments

Excised soybean roots were exposed to an aqueous solution of 1,3,5-trichlorobenzene. Effective equilibration was reached within 2.5 hr and the elimination rate constant was >4.1 hr⁻¹ (25).

Residues have been isolated from natural waters, sediments, fish tissues, vegetable oils and in urban air samples (26).

Environmental fate reviewed (26).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (27).

References

1. Hansch, C. et al *Medchem Project Issue No. 26* 1985, Pomona College, Claremont, CA, USA.
2. Konemann, W. H. *Quantitative Structure-Activity Relationships for Kinetics and Toxicity of Aquatic Pollutants and their Mixtures to Fish* 1979, Univ. Utrecht, Netherlands.
3. Hodson, P. V. et al *Environ. Toxicol. Chem.* 1988, **7**(6), 443-454.
4. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
5. Blum, D. J. W. et al *Res. J. Water Pollut. Control. Fed.* 1991, **63**(3), 198-207.
6. Niinomi, J. et al *Mie-Ken Kankō Kagaku Senta Kenkyū Hokok* 1989, (9), 53-60 (Japan.) (*Chem. Abstr.* **111**, 189142x).
7. Kirk, P. W. W. et al *Chemosphere* 1989, **128**(9-10), 1771-1784.
8. Worne, H. E. *Tijdschrift BECEWA* Liege, Belgium.
9. GEMS: Graphical Exposure Modeling System. *Fate of Atmospheric Pollutants* 1986, US EPA, Office of Toxic Substances, Washington, DC, USA.
10. Uyeta, M. et al *Nature* 1976, **264**, 583-584.
11. Fisel, P. et al *Fresenius Z. Anal. Chem.* 1984, **319**, 160-164.
12. Oliver, B. G. et al *Environ. Sci. Technol.* 1986, **18**, 903-908.
13. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
14. *Ind. Environ. Xenobiot.-Metab. Pharmacokinet. Org. Chem. Metals, Proc. Int. Conf. Prague, 1980* 1981, 389, Springer-Verlag, Berlin, Germany.
15. *Report UCRTL-13701 Natl. Tech. Inf. Ser.*, Washington, DC, USA.
16. Mohtashamipur, E. et al *Mutagenesis* 1987, **2**(2), 111-117.
17. Cote, M. et al *Drug Chem. Toxicol.* 1988, **11**(1), 11-28.
18. Rupa, D. S. *Bull. Environ. Contam. Toxicol.* 1988, **41**(5), 737-741.
19. Chu, I. et al *J. Environ. Sci. Health Part B* 1987, **B22**(4), 439-453.
20. Lenga, R. E. *The Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, Sigma-Aldrich, Milwaukee, WI, USA.
21. Klopman, G. et al *Mol. Toxicol.* 1987, **1**, 61-81.
22. Herven-Freund, S. L. et al *Environ. Health Perspect.* 1986, **69**, 59-65.
23. Parrini, M. et al *Boll.-Soc. Ital. Biol. Spec.* 1990, **66**(7), 709-716.

24. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
25. Kraaij, H. et al *Chemosphere* 1997, **34**(12), 2607-2620.
26. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1989, 1, 528-534, Lewis Publ., Chelsea, MI, USA.
27. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T244 2,3,4-trichloro-1-butene



$\text{C}_4\text{H}_5\text{Cl}_3$

Mol. Wt. 159.44

CAS Registry No. 2431-50-7

EINECS No. 219-397-9

RTECS No. EM 9046000

Physical properties

B. Pt. 157-160°C at 680 mmHg **Specific gravity** 1.3426 at 20°C

Solubility Organic solvents: chloroform

Occupational exposure

UN No. 2322 **HAZCHEM Code** 2Z **Conveyance classification** toxic substance

Supply classification toxic, dangerous for the environment

Risk phrases Harmful if swallowed – Toxic by inhalation – Irritating to eyes, respiratory system and skin –

Possible risk of irreversible effects – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R22, R23, R36/37/38, R40, R50/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Wear suitable protective clothing and gloves - In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S36/37, S45, S60, S61)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 341 mg kg⁻¹ (1).

LD₅₀ intragastric rat 350 mg kg⁻¹ (2).

Other effects

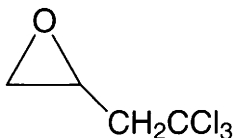
Any other adverse effects

A LD₅₀ dose intragastrically to rats caused toxic effects to the brain and liver which were more serious than effects to the heart and kidney (2).

References

1. *Cig. Sanit.* 1981, **46**(1), 92.
2. Petrosyan, F. R. et al *Biol. Zh. Arm.* 1987, **40**(8), 658-662 (*Chem. Abstr.* **108**, 144954k)

T245 trichlorobutylene oxide



$\text{C}_4\text{H}_5\text{Cl}_3\text{O}$

Mol. Wt. 175.44

CAS Registry No. 3083-25-8

Synonyms (2,2,2-trichloroethyl)oxirane; 1,1,1-trichloro-3,4-epoxybutane; 1,2-epoxy-4,4,4-trichlorobutane

EINECS No. 221-385-3

RTECS No. EK 3875000

Physical properties

B. Pt. 110°C at 100 mmHg Specific gravity 1.426 at 20°C

Mammalian & avian toxicity

Acute data

LD_{50} intravenous mouse 56 mg kg^{-1} (1).

Irritancy

Dermal (24 hr) rabbit 720 mg kg^{-1} caused severe irritation (2).

Genotoxicity

Salmonella typhimurium TA97, TA100 without metabolic activation positive, with metabolic activation negative; TA98, TA1535 with and without metabolic activation negative (3).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (4).

References

1. Report NX 0202d US Army Armament Research and Development Command, Chemical Systems Laboratory, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD, USA.
2. Olin Chemicals Data Sheet 1976, Industrial Development, New York, NY, USA.
3. Canter, D. A. et al *Mutat. Res.* 1986, **172**, 105-138.
4. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T246 trichloro(chloromethyl)silane



$\text{CH}_2\text{Cl}_4\text{Si}$

Mol. Wt. 183.92

CAS Registry No. 1558-25-4

Synonyms (chloromethyl)trichlorosilane

EINECS No. 216-316-9

RTECS No. VV 2200000

Uses Organic synthesis.

Physical properties

B. Pt. 117-118°C Flash point 69°C Specific gravity 1.4441 at 20°C

Mammalian & avian toxicity

Acute data

LD_{Lo} oral mouse 100 mg kg⁻¹ (1).
LC₅₀ (2 hr) inhalation mouse 30 mg m⁻³ (1).
LD_{Lo} dermal mouse 100 mg kg⁻¹ (1).
LD_{Lo} intraperitoneal mouse 100 mg kg⁻¹ (1).

Other effects

Other adverse effects (human)

Extremely destructive to tissue of the mucous membrane, upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema (2).

Other comments

Chemical safety information given (3).

References

1. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
2. Lenga, R. E. (Ed.) *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, 1, 813.
3. *Chemical Profile: Trichloro(chloromethyl)silane* 1985, US EPA, Washington, DC, USA

T247 1,1,1-trichloroethane



C₂H₃Cl₃

Mol. Wt. 133.40

CAS Registry No. 71-55-6

Synonyms methylchloroform; methyltrichloromethane; α-trichloroethane; trichloromethylmethane; Distillex DS1; Baltane; Ethana; Solvent 111; Tri-ethane

EINECS No. 200-756-3

RTECS No. KJ 2975000

Uses Industrial solvent for paints, inks, varnishes, correction fluid, dry cleaning agents. Metal cleaning and degreasing and in plastic mould cleaning. Additive to flammable solvents to raise flash point. Developer for printed circuit boards. Chemical intermediate.

Physical properties

M. Pt. -35°C (99.5% pure) B. Pt. 74-76°C Flash point none Specific gravity 1.3376 at 20°C with respect to water at 4°C Partition coefficient log P_{ow} 2.47 (1) Volatility v.p. 100 mmHg at 20°C; v.den. 4.6
Solubility Water: insoluble in water; absorbs some water. Organic solvents: acetone, benzene, carbon tetrachloride, diethyl ether, methanol

Occupational exposure

DE-MAK 200 ppm (1100 mg m⁻³)

FR-VME 300 ppm (1650 mg m⁻³)

JP-OEL 200 ppm (1100 mg m⁻³)

SE-LEVL 50 ppm (300 mg m⁻³)

UK-LTEL 200 ppm (1110 mg m⁻³)

US-TWA 350 ppm (1910 mg m⁻³)

FR-VLE 450 ppm (2500 mg m⁻³)

SE-STEL 90 ppm (500 mg m⁻³)

UK-STEL 400 ppm (2220 mg m⁻³)

US-STEL 450 ppm (2460 mg m⁻³)

UN No. 2831 HAZCHEM Code 2.2 Conveyance classification toxic substance

Supply classification harmful, dangerous for the environment

Risk phrases Harmful by inhalation – Dangerous for the ozone layer (R20, R59)

Safety phrases Restricted to professional users – Keep out of reach of children (if sold to general public) – Avoid contact with skin and eyes – Refer to manufacturer/supplier for information on recovery/recycling – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S24/25, S59, S61)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow, sheepshead minnow, bluegill sunfish 53-72 mg l⁻¹ (2-4).

Invertebrate toxicity

LC₅₀ (duration unspecified) *Philodina erythrophthalma* 162 mg l⁻¹ (5).

LC₅₀ (duration unspecified) *Colpoda* 305 mg l⁻¹ (5).

LC₅₀ (48 hr) *Daphnia magna* >530 mg l⁻¹ (6).

Bioaccumulation

Bluegill sunfish bioconcentration factor 9 (1).

Levels (in µg kg⁻¹) found in marine organisms collected from UK estuaries were: plankton 0.03-10.7; marine algae 10-25; fish 0.7-5 (flesh), 1-15 (liver); seal 0.2-4 (liver); 8-24 (blubber) (7).

Environmental fate

Degradation studies

Under methanogenic conditions at 35°C 100 µg l⁻¹ was degraded to 0.3 µg l⁻¹ in 8 wk, in the sterile controls no degradation occurred (8).

Reaction products include chloroethane and 1,1-dichloroethane; however, the latter product was produced by abiotic breakdown (9).

In sediment under anaerobic conditions it was completely degraded by 4-5 months; the major degradation product was 1,1-dichloroethane (10).

Degraded by a mixed anaerobic culture to methylene chloride (11).

In soil collected from just above the groundwater table no aerobic degradation of 1 mg l⁻¹ was measured (12). ≤110 mg l⁻¹ had no effect on the BOD value; 460 mg l⁻¹ halved the BOD value (5).

Bacterial cultures isolated from contaminated sites degraded 1,1,1-trichloroethane (13).

Abiotic removal

In aquatic systems volatilisation is the major route of removal; oxidation and hydrolysis do not play an important role in removal from water. 90% evaporation occurred after 60-80 min at 25°C, t_{1/2} 20 min (14).

1,1,1-trichloroethane was applied to columns containing sandy or sandy loam soils. 90 and 45%, respectively, of the applied solvent was lost via volatilisation (15).

In the troposphere it is oxidised by reaction with free hydroxyl radicals produced by the action of UV light to form trichloroacetaldehyde, which is then oxidised to trichloroacetic acid. For this oxidation a t_{1/2} of 6 yr has been estimated (16).

Adsorption and retention

Absorption by loam and sandy loam soils was characterised by a linear model; there was a greater affinity for the organic carbon-rich loam (17).

Mammalian & avian toxicity

Acute data

LD₅₀ oral guinea pig, mouse, rabbit, rat 8600, 9700, 10500, 11,000, 14,300 mg kg⁻¹, respectively (18).

LC₅₀ inhalation (6 hr) mouse, (7 hr) rat 13,410 and 14,250 ppm, respectively (19,20).

LD₅₀ dermal rabbit 15,800 mg kg⁻¹ (18).

LD₅₀ intraperitoneal mouse, dog 3700 and 5080 mg kg⁻¹, respectively (21-23).

Sub-acute and sub-chronic data

Schedule-controlled operant behaviour in inhalation Sprague-Dawley rats (100 min) 500-5000 ppm was studied. Inhalation of 1000 ppm slightly increased operant response rates whilst 2000, 3500, and 5000 ppm decreased operant response rates in a concentration and time-dependent manner. 1,1,1-Trichloroethane rapidly accumulated in the blood and brain in a concentration-dependent manner. The level in the brain was around twice the concentration found in the blood (24).

Oral (6 wk) rat 3.2-10 g kg⁻¹ 5 day wk⁻¹. No adverse effects were observed at 3.2 g kg⁻¹. 5.6 g kg⁻¹ for ♀ and 10 g kg⁻¹ ♂ caused 40% mortality with the survivors having decreased body weight. Mice fed 5.6 g kg⁻¹ 5 days wk⁻¹ had no increase in mortality (25).

Inhalation (30 day) rat 2700 mg m⁻³ 6 hr day⁻¹ 5 day wk⁻¹ caused a slight decrease in brain RNA levels, but had no effect on behaviour. 1750 mg m⁻³ for 30 days had no effect on brain lipids (25,26).

Inhalation (6 month) 2730 mg m⁻³, 7 hr day⁻¹, 5 day wk⁻¹ caused no adverse effect to rabbits, dogs, monkeys, rats or guinea pigs (27).

Inhalation (14 wk) mouse 5400 mg m⁻³ continuously caused marked liver changes, which included weight increase, moderate triacylglycerol accumulation and necrosis of individual hepatocytes (28).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, limited evidence of carcinogenicity to animals, IARC classification group 3 (29).

Inhalation (2 yr) Fischer 344 rat, B6C3F1 mouse 150, 500 or 1500 ppm 6 hr day⁻¹, 5 day wk⁻¹. Rats exposed to 1500 ppm had a significant decrease in body weight; slight microscopic hepatic lesions were observed at 6, 12 and 18 months, but not at the termination of the study. There were no toxic effects observed at lower doses in rats or at all doses in mice. There were no oncogenic effects seen in either mice or rats (30).

Gavage (78 wk) 2000 or 4000 mg kg⁻¹ day⁻¹ for wk 1-10; 3000 or 6000 mg kg⁻¹ day⁻¹ for wk 20-78. Each dose was administered 5 × wk⁻¹. After wk 78 the mice were fed a normal diet until wk 95. Treatment animals and controls had poor survival rates. Three high-dose group ♂s developed liver cell adenomas and one a hepatocellular carcinoma. This incidence of neoplasms was not statistically different from the controls (31).

Teratogenicity and reproductive effects

Oral mice 100, 300 or 1000 kg⁻¹ day⁻¹ in drinking water. In a two-generation study, no adverse effects to any aspects of reproduction were evident (32).

Oral rat 3, 10 or 30 mg l⁻¹ drinking water 14 days prior to co-habitation and at least 13 day after, there were no adverse effect to reproductive parameters (32).

Inhalation ♀ rat 11,340 mg m⁻³, 6 hr day⁻¹, 5 day wk⁻¹ for 2 wk prior to mating and/or 6 hr day⁻¹, 5 day wk⁻¹ for 20 days of gestation. No maternal toxicity was observed, but there was some evidence of foetotoxicity, viz. reduced foetal weight (group exposed during pregnancy only) and minor visceral and skeletal abnormalities (group exposed prior to and during pregnancy) (33).

Metabolism and toxicokinetics

Inhalation exposure of pregnant mice to 100 ppm for 1 hr showed concentrations in the placenta to be slightly lower than that in the blood (34).

Inhalation rat 370 or 2700 mg m⁻³. Absorption was time-dependent, and there was an initial uptake of >80% of the dose; during the 1st hr this decreased to 50%. The absorbed 1,1,1-trichloroethane was poorly metabolised (35).

Inhalation (16 month) rat 8100 mg m⁻³, 6 hr day⁻¹, 5 day wk⁻¹ did not result in significant tissue accumulation (36). Metabolites identified in rats included the glucuronide of 2,2,2-trichloroethanol, carbon dioxide, trichloroethanol and trichloroacetic acid, although the majority of the dose was excreted unchanged (37,38).

♂ Fischer 344 rats exposed dermally for 24 hr had a peak blood level of 3.4 µg ml⁻¹ within 4 hr (39).

Dermal guinea pig rapid absorption occurred with levels in the blood reaching 1.9 mg l^{-1} within 30 min (40,41). The calculated rate of absorption through skin is $6 \text{ } \mu\text{g min}^{-1}$ in guinea pigs (42). Inhalation (1 hr) dog 4.05, 8.1, or 10.8 g m^{-3} , the cumulative uptake was 2.5, 45, and 71 mg kg^{-1} , respectively. Arterial and venous blood concentrations did not reach steady state (43). Inhalation (6-8 hr) σ human 200-2000 mg m^{-3} , 20-40% inhaled was absorbed by the lungs (16). Dermal (occluded) human 15 ml, $16.2\text{-}27 \text{ mg m}^{-3}$ was measured in exhaled air (44). In a fatal case of poisoning in humans, 1,1,1-trichloroethane residues were detected in the bile, blood, brain, kidneys, liver and lungs, indicating it can also cross the blood-brain barrier (45). Humans exposed to $22\text{-}1890 \text{ mg m}^{-3}$ in air excreted 3-7% as metabolites in urine (16).

Irritancy

Dermal rabbit (4 hr) semi-occlusive dressing reported to be a skin irritant (46). 0.1 ml instilled into rabbit eye caused mild irritation (27,47). Dermal rabbit (24 hr) to shaved skin under an occlusive dressing caused moderate irritation (47). Exposure to 500 ppm for 3 hr caused eye irritation in humans (48).

Genotoxicity

Salmonella typhimurium TA100 with metabolic activation positive (49).
In vitro Chinese hamster ovary cells, chromosomal aberrations without metabolic activation positive, with metabolic activation equivocal; sister chromatid exchanges with and without metabolic activation equivocal (50).
In vitro mouse L5178Y lymphoma cells with metabolic activation equivocal, without negative (51).
In vitro rat, mouse hepatocytes unscheduled DNA synthesis negative (52).
Drosophila melanogaster sex-linked recessive lethals negative (53).
In vivo rat chromosomal aberrations negative (54).
In vivo mouse micronucleus test, dominant lethals negative (53,55).

Other effects

Other adverse effects (human)

Occupationally exposed workers with long-term repetitive high exposures were found to have significant deficits in memory, intermediate memory, rhythm, speed, and ocular components of balance (56). Exposure to 500 ppm for 3 hr caused headaches (48).

Any other adverse effects

In rats (dose unspecified) causes central nervous system depression. Following inhalation for 14 wk, mice have developed hepatotoxicity (57,58).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (59). Data used in setting UK occupational exposure limit summarised (60). Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorines: guide level $1 \text{ } \mu\text{g l}^{-1}$; maximum admissible concentration $100 \text{ } \mu\text{g l}^{-1}$ (61).

Other comments

It is estimated (in 1978) that 97.3% of the 1,1,1-trichloroethane used in the USA was released into the environment, 85% to air, 1% to water and ~10% is disposed of as waste. Most was released during use, rather than manufacture. Once in the stratosphere it causes ozone depletion by the release of reactive chlorine atoms and also contributes to global warming (16). The London Conference of the Montreal Protocol (June, 1990) agreed to discontinue its use (16). Genotoxicity testing with *Escherichia coli* in the SOS-chromotest found that the methodology of this test was unsuitable for assessing the genotoxic potential of volatile compounds, including 1,1,1-trichloroethane (62). Reviews on human health effects, experimental toxicology, physico-chemical properties listed (63). Autoignition temperature 537°C .

References

1. Veith, G. D. et al *Proceedings of the Third Annual Symposium on Aquatic Toxicology* 1980, 116-129, American Society for Testing and Materials (ASTM STP No. 707), Philadelphia, PA, USA.
2. Konemann, W. H. *Quantitative structure-activity relationships for kinetics and toxicity of aquatic pollutants and their mixtures in fish* 1979, Univ. Utrecht, Netherlands.
3. Heitmüller, P. T. et al *Bull. Environ. Contam. Toxicol.* 1981, **27**, 596-604.
4. Buccafusco, R. J. et al *Bull. Environ. Contam. Toxicol.* 1981, **26**, 446.
5. Inamouri, Y. et al *Water Sci. Technol.* 1989, **21**(12), 1887-1890.
6. LeBlanc, G. A. *Bull. Environ. Contam. Toxicol.* 1980, **24**, 684-691.
7. Pearson, C. R. *The Handbook of Environmental Chemistry* 1982, Vol. 3, Part B, 69-88, Hutzinger, D. ed., Springer-Verlag, Berlin, Germany.
8. Bouwer, E. J. et al *Appl. Environ. Microbiol.* 1983, **45**, 1286-1294.
9. Kleck, A. G. M. et al *Environ. Toxicol. Chem.* 1990, **9**, 1437-1451.
10. Parsons, F. et al *J. Am. Water Works Assoc.* 1985, **77** 52-59.
11. Vargas, C. et al *J. Water Pollut. Control Fed.* 1987, **59**(11), 964-968.
12. Wilson, J. T. et al *Dev. Ind. Microbiol.* 1983, **247**, 125-233.
13. Kaester, M. *DECHEMA Biotechnol. Conf.* 1989, **3**(Pt. B), 909-912.
14. Dilling, W. L. et al *Environ. Sci. Technol.* 1975, **9**, 833-838.
15. Drake, R. J. *Fate of Methylene Chloride and 1,1,1-trichloroethane in unsaturated, biologically active soils* 1987, Dissertation, Univ. Massachusetts, USA.
16. *IPCS Environmental Health Criteria No. 136* 1992, World Health Organisation, Geneva, Switzerland.
17. Ollinger, W. M. et al *Proc. Ind. Waste Conf.* 1987 Publ. 1988, **42nd**, 781-785.
18. Torkelson, T. R. et al *Am. Ind. Hyg. Assoc. J.* 1958, **19**, 353-362.
19. Adams, E. M. et al *Arch. Ind. Hyg.* 1950, **1**, 225-236.
20. Gradiski, I. D. et al *Arch. Mol. Prof. Med. Trav. Secur. Soc.* 1978, **39**, 249-252.
21. Gradiski, I. D. et al *J. Eur. Toxicol.* 1974, **7**, 247-254.
22. Klaassen, C. D. et al *Toxicol. Appl. Pharmacol.* 1967, **10**, 119-131.
23. Klaassen, C. D. et al *Toxicol. Appl. Pharmacol.* 1966, **9**, 139-151.
24. Warren, D. A. et al *Neurotoxicol. Teratol.* 1998, **20**(2), 143-153.
25. Salolainen, H. et al *Arch. Toxicol.* 1977, **38**, 29-237.
26. Kyrklund, T. et al *Scand. J. Work, Environ. Health* 1988, **14**, 91-94.
27. Torkelson, T. R. et al *Am. Ind. Hyg. Assoc. J.* 1958, **19**, 353-362.
28. McNutt, N. S. et al *Lab. Invest.* 1975, **5**, 624-654.
29. *IARC Monograph* 1987, **Suppl. 7**, 73.
30. Quast, J. F. et al *Fundam. Appl. Toxicol.* 1988, **11**(4), 611-625.
31. *National Cancer Institute Report (NIH) 77803* 1977, US Department of Health, Education and Welfare, Washington, DC, USA.
32. George, J. D. et al *Fundam. Appl. Toxicol.* 1989, **13**, 641-651.
33. York, R. G. et al *J. Toxicol. Environ. Health* 1982, **9**, 251-266.
34. Shimada, Y. *Okayama Igasskai Zasshi* 1988, **100**(1/2), 147-153 (Japan.) (*Chem. Abstr.* **109**, 124063m).
35. Dallas, C. E. et al *Toxicol. Appl. Pharmacol.* 1989, **98**, 385-897.
36. Schumann, A. M. et al *Toxicol. Appl. Pharmacol.* 1982, **62**, 390-401.
37. Hake, C. L. et al *Arch. Environ. Health* 1960, **177**, 101-105.
38. Eben, A. et al *Arch. Toxicol.* 1974, **31**, 233-242.
39. Morgan, D. L. et al *Environ. Res.* 1991, **55**(1), 51-63.
40. Jakobson, M. et al *Khim. Drev.* 1980, **1**, 37-46.
41. Jakobson, I. et al *Toxicol. Appl. Pharmacol.* 1982, **63**, 181-187.
42. *1,1,1-Trichloroethane* 1984, Health and Safety Executive, London, UK.
43. Hobard, T. et al *Jpn. J. Ind. Health* 1982, **24**, 599-607.
44. Nakaaki, K. et al *J. Sci. Labour* 1980, **56**, 1-9.
45. Caplan, Y. H. et al *Clin Toxicol.* 1976, **9**, 69-74.
46. Van Beek, L. *TNO Report No. U89.265* 1990, Project No. B86-0927, Organisation for Applied Scientific Research, Apeldoorn, The Netherlands.
47. Diprat, P. et al *Eur. J. Toxicol. Environ. Hyg.* 1976, **9**, 171-177.
48. Verscheuren, K. (Ed.) *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, Van Nostrand Reinhold, New York, NY, USA.

49. Simmon, V. F. et al *Progress in Genetic Toxicology* 1977, 249-258, Scott, D. et al (Ed.), Elsevier/North Holland, Amsterdam, Netherlands.
50. Galloway, S. M. et al *Environ. Mol. Mutagen.* 1987, **10**, 1-175.
51. Myhr, B. C. et al *Environ. Mol. Mutagen.* 1988, **13**, 103-194.
52. Althaus, F. R. et al *Cancer Res.* 1982, **42**(8), 3010-3015.
53. Gocke, E. et al *Mutat. Res.* 1981, **90**, 91-109.
54. Quast, J. F. et al *Report* 1978, Dow Chemical Co., Midland, Michigan, USA.
55. Lane, R. W. et al *Toxicol. Appl. Pharmacol.* 1982, **63**, 409-421.
56. Kelafant, G. A et al *Am. J. Ind. Med.* 1994, **25**(3), 439-446.
57. Adams, E. M. et al *Arch. Ind. Hyg.* 1950, **1**, 225-236.
58. McNutt, N. S. et al *Lab. Invest.* 1975, **32**, 642-654.
59. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
60. *Occupational Exposure Limits: Criteria Document Summaries* 1993, HMSO, London, UK.
61. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
62. Mersch-Sundermann, V. et al *Zentralbl. Hyg. Umweltmed.* 1989, **189**(3), 266-261.
63. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T248 1,1,2-trichloroethane



$\text{C}_2\text{H}_3\text{Cl}_3$

Mol. Wt. 133.40

CAS Registry No. 79-00-5

Synonyms 1,2,2-trichloroethane; vinyl trichloride

EINECS No. 201-166-9

RTECS No. KJ 3150000

Uses Solvent for natural resins, fats, alkaloids, waxes. Manufacture of 1,1-dichloroethylene.

Physical properties

M. Pt. -36.7°C B. Pt. 114°C Specific gravity 1.442 at 20°C with respect to water at 4°C

Volatility v.p. 44 mmHg at 35.2°C ; v.den. 4.63

Solubility Organic solvents: miscible with diethyl ether, ethanol

Occupational exposure

DE-MAK 10 ppm (55 mg m^{-3})

JP-OEL 10 ppm (55 mg m^{-3})

US-TWA 10 ppm (55 mg m^{-3})

UN No. 2810

Supply classification harmful

Risk phrases Harmful by inhalation, in contact with skin and if swallowed (R20/21/22)

Safety phrases Restricted to professional users – Keep out of reach of children (if sold to general public) – Keep container in a well ventilated place (S2, S9)

Ecotoxicity

Fish toxicity

LC_{50} (96 hr) fathead minnow 0.082 g l^{-1} (1).

LC_{50} (7-14 day) guppy 0.094 g l^{-1} (1).

LC_{50} (96 hr) American flagfish 89.1 mg l^{-1} (2).

Invertebrate toxicity

EC₅₀ (5 min) *Photobacterium phosphoreum* 106 ppm Microtox test (3).

LOEC (reproduction) *Scenedesmus quadricauda* 430 mg l⁻¹ (duration unspecified) (4).

LC₅₀ (48 hr) *Daphnia magna* 18 mg l⁻¹ (5).

Bioaccumulation

Confirmed to be low / non-bioaccumulative (6).

Environmental fate

Adsorption and retention

Soil sorption coefficient K_{om} 1.87 (7).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, dog, rat 378-836 mg kg⁻¹ (8-10).

LC_{Lo} (4 hr) inhalation rat 2000 ppm (11).

LC_{Lo} (4.5 hr) inhalation cat 13,100 mg m⁻³ (12).

LD₅₀ dermal rabbit 5377 mg kg⁻¹ (10).

LD₅₀ intraperitoneal dog, mouse 450, 494 mg kg⁻¹, respectively (13,14).

LD₅₀ subcutaneous mouse 277 mg kg⁻¹ (15).

LD_{Lo} intravenous dog 95 mg kg⁻¹ (16).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, limited evidence for carcinogenicity to animals, IARC classification group 3 (17).

Subcutaneous (2 yr) Sprague-Dawley rats 0.002 or 0.006 mg wk⁻¹. There was no significant increase in benign mesenchymal and epithelial tumours, the high-dose group had a higher incidence of sarcomas (18).

The National Toxicology Program tested rats and mice via gavage. There was no evidence of carcinogenicity in rats. There was positive evidence of carcinogenicity in ♂ and ♀ mice as characterised by hepatocellular carcinomas and pheochromocytoma of the adrenal gland (19).

Teratogenicity and reproductive effects

Gavage mice day 8-12 of gestation (dose unspecified) was not embryotoxic or teratogenic (20).

Metabolism and toxicokinetics

0.0053 or 0.0213 mg injected into ♂ Wistar rats, by 24 hr the metabolites thiodiglycolic acid and hydroxyethyl mercapturic acid were detected in urine (18).

Intraperitoneal mouse 0.1-0.2 g kg⁻¹ of [¹⁴C]-1,1,2-trichloroethane. 73-87% was found in urine and 16-22% was expired (40% unchanged and 60% as carbon dioxide). Three metabolites were identified in urine: chloroacetic acid, S-carboxymethylcysteine, and thiodiacetic acid. Small amounts of glycolic acid, 2,2-dichloroethanol, 2,2,2-trichloroethanol, oxalic acid, and trichloroacetic acid were detected (21).

Irritancy

Caused skin irritation in guinea pigs (details unspecified) (22).

In humans it is an eye and mucous membrane irritant. Dermal contact produces cracking and erythema (23).

Genotoxicity

Salmonella typhimurium TA1535 with and without metabolic activation negative (24).

In the *in vivo-in vitro* hepatocyte DNA repair assay in mouse liver it was a potent inducer of S-phase synthesis but not unscheduled DNA synthesis (25).

♂ Osborne Mendel rats, rat liver foci assay for tumour initiating and promoting activity, induced a significant increase in the GGT⁺ foci (26).

Other effects

Other adverse effects (human)

It has narcotic action at low concentrations. Long-term exposure to the vapour produces chronic gastric symptoms, fat deposition in the kidney and lung damage (23).

Any other adverse effects

Administration (route unspecified) to mice, there was a decrease in liver ATP, an increase in liver triglyceride, a decrease in plasma triglyceride and an increase in GPT, these effects were greater than with the 1,1,1-isomer (27).

It depresses the central nervous system, is hepatotoxic and induces kidney damage in mice (28).

An LD₁₀ administration to mice caused hepatic dysfunction; higher doses caused centrilobular necrosis (29).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (30).

Other comments

The *Escherichia coli* SOS-chromotest was found not to be valid for testing volatile compounds (31).

1,1,2-trichloroethane is considered to be considerably more toxic than the 1,1,1-isomer (32).

Toxicity and health effects reviewed (33).

Production, uses, physical properties, toxicity, carcinogenicity reviewed (28).

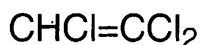
Reviews on human health effects, experimental toxicology, physico-chemical properties listed (34).

References

1. Abernethy, S. et al *Environ. Toxicol. Chem.* 1988, 7(6), 469-48.
2. Smith, A. D. et al *Arch. Environ. Contam. Toxicol.* 1991, 20 94-102.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, 26(3), 94-102.
4. Bringmann, G. et al *Water Res.* 1988, 14, 231-241.
5. LeBlanc, G. A. *Bull. Environ. Contam. Toxicol.* 1980, 24, 684-691.
6. *The list of existing chemical substances tested on biodegradability by microorganisms or bioaccumulation in fish body* 1987, Chemicals Inspection and Testing Institute, Japan.
7. Sabljic, A. *QSAR Environ. Toxiol. Proc. Int. Workshop, 2nd 1986 Publ.* 1987, 309-332, Kaiser, K. L. E. (Ed.), Reidel, Dordrecht, Netherlands.
8. *Drug Chem. Toxicol.* 1985, 8, 333.
9. *Am. J. Hyg.* 1932, 16, 325.
10. Smyth, H. F. et al *Am. Ind. Hyg. Assoc. J.* 1969, 30, 470.
11. *J. Ind. Hyg.* 1932.
12. *Arch. Hyg. Bakteriolog.* 1936, 116, 131.
13. *Toxicol. Appl. Pharmacol.* 1967, 10, 119.
14. *Toxicol. Appl. Pharmacol.* 1966, 9, 139.
15. *J. Pharmacol. Exp. Ther.* 1958, 123, 224.
16. *Quart. J. Pharm. Pharmacol.* 1934, 7, 205.
17. *IARC Monograph* 1987, **Suppl.** 7, 73.
18. Norpoth, K. et al *J. Cancer Res. Clin. Oncol.* 1988, 114(2), 158-162.
19. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-74, NIEHS, Research Triangle Park, NC, USA.
20. Seiderberg, J. M. et al *Teratog., Carcinog., Mutagen.* 1987, 7(1), 17-28.
21. Yllner, S. *Acta Pharmacol. Toxicol.* 1971, 30 248-256.
22. Kroneji, T. et al *Acta Pharmacol. Toxicol.* 1977, 41, 298-305.
23. Hardie, D. W. F. *Encyclopedia of Chemical Technology* 2nd ed., 1964, 5, 1571-159, Kirk, R. E. et al (Ed.), John Wiley & Sons, New York, NY, USA.
24. Rannug, U. et al *Chem.-Biol. Interact.* 1978, 20, 1-16.
25. Mirsalis, J. C. et al *Environ. Mol. Mutagen.* 1989, 14(3), 155-164.
26. Milman, H. A. et al *Ann. N.Y. Acad. Sci.* 1988, 534, (Living Chem. World), 521-530.
27. Takahara, K. *Okayama Igakkai Zasshi* 1986, 98(11/12), 1099-1109 (Japan.) (*Chem. Abstr.* 107, 2220y).
28. *IARC Monograph* 1979, 20, 533-543.
29. Klaassen, C. D. et al *Toxicol. Appl. Pharmacol.* 1966, 9, 139-151.

30. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations 1991*, HMSO, London, UK.
31. Mersch-Sundermann, V. et al *Zentralbl. Hyg. Umweltmed.* 1989, **18993**, 26-271 (Ger.) (*Chem. Abstr.* **112**, 193568d).
32. *Gov. Rep. Announce. Index (U.S.)* 1989, **80**(18).
33. *Gov. Rep. Announce. Index (U.S.)* 1990, **90**(12).
34. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T249 trichloroethylene



C_2HCl_3

Mol. Wt. 131.39

CAS Registry No. 79-01-6

Synonyms trichloroethene; 1,1,2-trichloroethylene; ethinyl trichloride; ethylene trichloride; chlorylen; Distillex DS2; Altene; Triklone; Triclene; Trineu

EINECS No. 201-167-4

RTECS No. KX 4550000

Uses Industrial solvent used to dissolve fats, waxes, oil, rubber paint, varnish, cellulose esters and ethers. Manufacture of organic chemicals and pharmaceuticals.

Physical properties

M. Pt. -84.8°C **B. Pt.** 86.7°C **Flash point** none **Specific gravity** 1.4649 at 20°C with respect to water at 4°C

Partition coefficient $\log P_{ow}$ 2.42 (1) **Volatility** v.p. 20 mmHg at 0°C; v.den. 4.53

Solubility Water: 1.100 mg l⁻¹ at 25°C. Organic solvents: miscible with chloroform, diethyl ether, ethanol

Occupational exposure

FR-VME 75 ppm (405 mg m⁻³)

FR-VLE 200 ppm (1080 mg m⁻³)

JP-OEL 50 ppm (270 mg m⁻³)

SE-LEVL 10 ppm (50 mg m⁻³)

SE-STEL 25 ppm (140 mg m⁻³)

UK-LTEL MEL 100 ppm (550 mg m⁻³)

UK-STEL MEL 150 ppm (820 mg m⁻³)

US-TWA 50 ppm (269 mg m⁻³)

US-STEL 100 ppm (537 mg m⁻³)

UN No. 1710 **HAZCHEM Code** 2Z **Conveyance classification** toxic substance

Supply classification harmful

Risk phrases Possible risk of irreversible effects – Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R40, R52/53)

Safety phrases Keep out of reach of children (if sold to general public) – Do not breathe vapour – Wear suitable protective clothing and gloves – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S23, S36/37, S61)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow 0.045 g l⁻¹ (2).

LC₅₀ (7-14 day) guppy 0.132 g l⁻¹ (2).

LC₅₀ (9 hr) sheepshead minnow 52 mg l⁻¹ (3).

LC₅₀ (96 hr) American flag fish 3.1 mg l⁻¹ (4).

Invertebrate toxicity

LC₅₀ *Philodina erythrophthalma*, *Aelosomas hemprichi*, *Colpoda* 92, 47, 75 mg l⁻¹, respectively (5).

EC₅₀ (5-30 min) *Photobacterium phosphoreum* 176 pm Microtox test (6).

Toxicity threshold (cell multiplication inhibition) *Microcystis aeruginosa*, *Pseudomonas putida*, *Scenedesmus quadricauda*, *Entosiphon sulcatum* 63, 65 >1000 and 1200 mg l⁻¹, respectively (7).

LC₁₀₀ (40 hr) *Daphnia* sp. 600 mg l⁻¹, no effect concentration 100 mg l⁻¹ (7).

Toxicity to other species

LC₅₀ (48 hr) clawed toad, Mexican axolotl 45, 48 mg kg⁻¹, respectively (8).

Bioaccumulation

Marine organisms from Liverpool bay had tissue concentrations of 3-100 ng g⁻¹ wet weight (9).

Levels found in marine organisms were: invertebrates, fish muscle, sea-bird eggs, seal fat 1, 10, 50 and 50 µg kg⁻¹ wet weight, respectively (9).

Environmental fate

Anaerobic effects

Three unsaturated soils containing indigenous methanotrophs which were stimulated by exposure to a methane/air atmosphere degraded 1,2-dichloroethane faster than trichloroethylene, with chloroform being degraded the slowest. Zero-order rate constants for the 3 solvents for the conversion into carbon dioxide were in the order of 0.05-1.4 µg solvent g⁻¹ day⁻¹ (10).

Degradation studies

Trichloroethylene was degraded by *Pseudomonas putida* strains F1 and B5 derived from groundwater via a *meta* fission aromatic degradative pathway (11).

Bacterial cultures isolated from contaminated sites degraded trichloroethylene (12).

Degradation by fresh water sediment system resulted in the formation of chloroethane, *cis*- and *trans*-1,2-dichloroethene and dichloromethane (13).

Under methanogenic conditions, enrichment cultures of trichloroethylene-degrading microorganisms were able to completely dechlorinate the compound to ethylene; there was no significant conversion to carbon dioxide (14).

Abiotic removal

Chemical degradation in sealed bottles t_{1/2} 2.5 yr (9).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 4.92 ml kg⁻¹ (15).

LD₅₀ oral mouse 2402 mg kg⁻¹ (16).

LD_{Lo} oral cat, rabbit 5864 and 7330 mg kg⁻¹, respectively (16,17).

LC₅₀ (1 hr), (4 hr) inhalation rat 25,700 ppm, 8000 ppm, respectively (18,15).

LC₅₀ (4 hr) inhalation mouse 8450 ppm (19).

LD₅₀ subcutaneous dog, rabbit 150 and 1800 mg kg⁻¹, respectively (17,20).

LD₅₀ intravenous mouse 33.9 mg kg⁻¹ (21).

LD_{Lo} intravenous dog 150 mg kg⁻¹ (22).

LD₅₀ intraperitoneal dog 1900 mg kg⁻¹ (23).

Sub-acute and sub-chronic data

Oral (13 wk) rat 125-2500 mg kg⁻¹ ♂, 625-1000 mg kg⁻¹ ♀ 5 × wk. All rats survived, ♂ receiving 2000 mg kg⁻¹ had a 24% decrease in body weight. High-dose animals had minimal/mild cytomegaly and karyomegaly of the renal tubular epithelial cells in the inner cortex (24).

Inhalation (5 day) ♂ Swiss Webster mouse 54,000 mg m⁻³ for 4 hr day⁻¹. NADPH cytochrome *c* reductase activity was decreased in the lungs, but increased in the liver. In the lungs there were platelet thrombi, and vacuolisation of bronchial epithelial cells (23).

Inhalation (45 day) rabbit 15,000 mg m⁻³ 4 hr day⁻¹, 6 days wk⁻¹ developed severe normocytic anaemia, leucopenia and thrombocytopenia caused by toxic effects on the bone marrow (25).

Intraperitoneal administration, 3 doses of 3330 mg kg⁻¹ on alternate days. No morphological changes were observed in the liver, but there was an increase in hepatic microsomal NADPH cytochrome *c* reductase activity (23).

CD-1 mice exposed to 450 ppm trichloroethylene 6 hr day⁻¹ 5 days wk⁻¹ for 2 wk showed vacuolation of lung Clara cells. The damage observed was caused by accumulation of chloral, caused by high rates of trichloroethylene metabolism (26).

Carcinogenicity and chronic effects

Insufficient evidence for carcinogenicity to humans, limited evidence for carcinogenicity to animals, IARC classification group 3 (27).

Inhalation (lifetime study) 100 or 600 ppm 7 hr day⁻¹ 5 day wk⁻¹ Swiss mice for 78 wk and Sprague-Dawley rats 104 wk. Under these conditions it appears to be carcinogenic, especially to ♂ mice, and is characterised by a dose-related increase in Leydig cell tumours in ♂ rats and the onset of renal tubules adenocarcinomas at the highest doses (28).

Gavage (18 month) rat, 549 or 1097 mg kg⁻¹ 5 × wk⁻¹; ♂ mice 1169 or 2339 mg kg⁻¹ 5 × wk⁻¹; ♀ mice 869 or 1739 mg kg⁻¹ 5 × wk⁻¹. Hepatocellular carcinomas were not seen in rats. In mice 30% of low-dose animals and 44.5% of the high-dose animals developed hepatocellular carcinomas (controls 2.5%) (29).

Gavage (lifetime study) rat 50 or 250 mg kg⁻¹ 4 or 5 × wk⁻¹ for 1 yr did not indicate a carcinogenic effect (30).

Inhalation (18 month) rat, mouse, Syrian hamster 100 or 500 ppm 6 hr day⁻¹ 5 day wk⁻¹, no indication of increased carcinogenicity (31).

Teratogenicity and reproductive effects

0.31-3.29 mg injected into chick eggs on days 1 and 2 of embryogenesis caused embryotoxicity, growth defects and morphological anomalies (32).

Inhalation mouse 1620 mg m⁻³ for 7 hr on days 6-15 of gestation, there were no foetotoxic or teratogenic effects (33).

Gavage ♂ rat 10, 100 or 1000 mg kg⁻¹ 5 day wk⁻¹ for 6 wk. No spermatotoxic effects. Copulatory behaviour was initially diminished by narcotic properties, but was normal by the 5th wk (34).

Metabolism and toxicokinetics

Dermal ♂ Fischer 344 rats exposed dermally had a peak blood level of 11-16 µg ml⁻¹ within 4 hr (35).

Pregnant mice exposed (route unspecified) to 500 ppm for 1 hr. Trichloroethylene was able to cross the placenta; concentrations were slightly higher in the placenta than in the blood (36).

In mammals, uptake is high during the initial inhalation exposure. It then declines until an equilibrium is reached between uptake by the blood and release from the blood to tissues and metabolism. After this equilibrium is reached the level of uptake remain constant for the rest of the exposure time (37,38).

In mammals, metabolism is mainly in the liver and is by the mixed-function oxidase enzyme system and is dependent on cytochrome P₄₅₀. The major metabolites are free and conjugated trichloroethanol and trichloroacetic acid; minor metabolites include 2-hydroxyacetyethanolamine and oxalic acid (39).

Trichloroethylene is metabolised to a small extent (< 0.01% of dose) via conjugation with glutathione to S-(1,2-dichlorovinyl)-L-cysteine (DCVC), which is a bacterial mutagen and nephrotoxin activated by the renal enzyme β-lyase. The authors suggest, however, that DCVC is probably not involved in the renal toxicity and subsequent tumour development seen in rats exposed to trichloroethylene (40).

Irritancy

Dermal rabbit (24 hr) 500 mg caused severe irritation, 20 mg instilled into rabbit eye (24 hr) caused moderate irritation (41).

160 ppm caused eye irritation in humans (42).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535 with and without metabolic activation negative, when in vapour phase and when stabilised with oxirane (43).

Escherichia coli WP2s (λ) microscreen assay without metabolic activation negative, with metabolic activation positive (44).

In vitro Chinese hamster ovary cells with and without metabolic activation weakly positive for sister chromatid exchanges; chromosomal aberrations with and without metabolic activation negative (45).

Aspergillus nidulans classified as a DNA damaging agent (46).

In vivo produced DNA strand breaks in rats livers (47).

In vivo occupationally exposed workers did not have an increase in sister chromatid exchanges in their lymphocytes (48).

Other effects

Other adverse effects (human)

Clinical examinations of three groups of people exposed to trichloroethylene (TCE) in well water are summarised. A high rate of cognitive deficits of the type seen in patients with central nervous system dysfunction attributable to solvent exposure was seen. A clear developmental trend was also seen. Subjects who were young at the time of TCE exposure showed a wider variety of cognitive deficits than those who were already adults (49).

Exposure can cause headache, sluggishness, dulling of senses, dizziness and nausea. At narcotic doses, vomiting may occur (39).

Organ systems reported to be affected by excessive exposure are central nervous system, liver, kidney, lung, heart and skin (50).

2500-6000 ppm is narcotic to humans (42).

Eighty-five workers exposed to trichloroethylene (TCE) in an electronics factory were examined for adverse effects on spermatogenesis. Semen analysis included volume, sperm density, viability, motility and morphology. Urine was analysed for the trichloroacetic acid metabolite. Workplace air was monitored for trichloroacetic acid (TCA). The mean environmental TCE level ranged between 9 and 131 ppm and the mean urine TCA ranged between 0.3 and 136.4 mg g⁻¹. The majority of the workers had normal sperm volume (71.8%), density (88.2%), and motility (64.7%). However, the subjects had a low percentage of normal sperm morphology. There were no significant differences in the mean sperm parameters among the "high exposure" (urine TCA ≤25 mg g⁻¹ creatinine) and "low exposure" (urine TCA ≤25 mg g⁻¹ creatinine) groups, except for sperm density. Prevalence rate ratios of hyperzoospermia were higher with increasing urine TCA levels compared the "low exposure" group, suggesting a dose-response with relationship (51).

A 58-yr-old man fell head first into a trichloroethylene reservoir bath during maintenance degreasing and ingested the solvent. He was admitted to hospital in a coma, with chemical burns and pneumonia. These symptoms gradually subsided. Blood and urine were analysed for trichloroethylene, trichloroethanol and trichloroacetic acid concentrations. Eight hours after the accident concentrations were 31.4 µg ml⁻¹, 16.5 µg ml⁻¹ and 79.5 µg ml⁻¹, respectively. The kinetics of trichloroethylene and its metabolites in blood and urine were in slight agreement with the results following inhalation exposure previously reported in the literature (52).

Any other adverse effects

In mice, a single dose of 2000 mg kg⁻¹ caused significant damage to the Clara cells of the bronchiolar epithelium within 24 hr (53).

The metabolites of trichloroethylene, trichloroacetate and dichloroacetate were capable of inducing tumours at a lower dose with a shorter latency than the parent compound in B6C3F1 mice. It is suggested that trichloroacetate is primarily responsible for the hepatocarcinogenic effects of trichloroethylene (54).

Mice were given 4.1 µg via intraperitoneal injection and sacrificed between 0.5 and 120 hours post-treatment. Binding of trichloroethylene to liver protein and DNA was measured using accelerator mass spectrometry. The highest level of protein binding (2.4 ng g⁻¹ protein) was observed at 1 hr post-treatment, followed by a rapid decline. This may indicate instability of the adducts and/or rapid turnover of liver proteins. DNA binding was biphasic, with the first peak (75 pg g⁻¹ DNA) at 4 hours. The highest binding was observed between 24 and 72 hours (120 pg g⁻¹) (55).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (56).

Data used in setting UK occupational exposure limit summarised (57).

Other comments

NIOSH has designated trichloroethylene an ototoxin. It can cause hearing loss, ringing in the ears or total deafness and its toxicity can be exacerbated by combined exposure to noise (58).

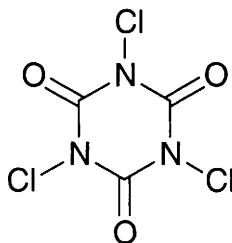
Photoluminescent and *Daphnia* tests for chlorinated solvents reviewed (59).
 Production, uses, toxicity and environmental effects reviewed (39).
 Toxicity, production, and use reviewed (60).
 Reviews on human health effects, experimental toxicology, physico-chemical properties listed (61).

References

1. Banerjee, S. et al *Environ. Sci. Technol.* 1980, **14**, 1227-1229.
2. Abernethy, S. G. et al *Environ. Toxicol. Chem.* 1988, **7**, 469-481.
3. Ward, G. S. et al *Bull. Environ. Contam. Toxicol.* 1986, **37**(6), 830-836.
4. Smith, A. D. et al *Arch. Environ. Contam. Toxicol.* 1991, **20**, 94-102.
5. Inamori, Y. et al *Water Sci. Technol.* 1989, **21**(12), 1887-1890.
6. Kaiser, K. L. E. *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
7. Bringmann, G. et al *Water Res.* 1980, **14**, 231-241.
8. Sloof, W. et al *Bull. Environ. Contam. Toxicol.* 1980, **24**, 397-403.
9. Pearson, C. R. et al *Proc. R. Soc. London: B* 1975, **189**, 305332.
10. Speitel, G. F. et al *J. Environ. Eng. (N. Y.)* 1991, **117**(5), 541-558.
11. Nelson, M. J. K. et al *Patent Application Eur. Pat. Appl.* EP 289,350 (Cl. C02F3/34), 02 Nov. 1988, US Appl. 44,213, 30 Apr. 1987, (*Chem. Abstr.* **110**, 44715t).
12. Kaestner, M. *DECHEMA Biotechnol. Conf.* 1989, **3**(Pt. B), 909-912.
13. Parsons, F. et al *J. Am. Water Works Assoc.* 1984, **76**(2), 56-59.
14. Freedman, D. L. et al *Appl. Environ. Microbiol.* 1989, **55**(9), 214-215.
15. Smyth, H. F. et al *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 470.
16. NTIS Report AD-A080-636, Natl. Tech. Inf. Ser., Springfield, VA, USA.
17. *Handbook of Toxicology* 1959, **5**, 76.
18. *Toxicol. Appl. Pharmacol.* 1977, **42**, 417.
19. *Acta Pharmacol. Toxicol.* 1953, **9**, 303.
20. *Quart. J. Pharm. Pharmacol.* 1934, **7**, 205.
21. *Summary Tables of Biological Tests* 1954, **6**, 141, National Research Council Chemical-Biological Coordination Center, Washington, DC, USA.
22. *Toxicol. Appl. Pharmacol.* 1967, **10**, 119.
23. Lesis, G. D. et al *Gen. Pharmacol.* 1984, **15**(2), 139-144.
24. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-243, NIEHS, Research Triangle Park, NC, USA.
25. Muzza, U. et al *Folia Med.* 1967, **50**, 318-324.
26. Green, T. et al *Fundam. Appl. Toxicol.* 1997, **37**(2), 125-130.
27. *IARC Monograph* 1987, **Suppl. 7**, 73.
28. Maltoni, C. et al *Ann. N. Y. Acad. Sci.* 1988, **534**(Living Chem. World), 316-342.
29. *National Cancer Institute Technical Report* 1976, Series No. 2 DHEW (NIH) Publ. 76-802; NTIS Pub. No. PB-264122, Natl. Tech. Inf. Serv., Springfield, VA, USA.
30. Maltoni, C. et al *Osp. Vita.* 1977, **4**, 108-110.
31. van Duuren, B. L. et al *J. Natl. Cancer Inst.* 1979, **63**, 1433-1439.
32. Bross, G. et al *Toxicology* 1983, **28**, 283-294.
33. Schwetz, B. A. et al *Toxicol. Appl. Pharmacol.* 1975, **32**, 84-94.
34. Zenick, H. et al *Toxicology* 1984, **31**, 237-250.
35. Morgan, D. L. et al *Environ. Res.* 1991, **56**(1), 51-63.
36. Shamada, Y. *Okayama Igakkai Zasshi* 1988, **100**(1/2), 147-153.
37. Fernandez, J. G. et al *Arch. Mol. Prof. Med. Trav. Secur. Soc.* 1975, **36**(7-8), 397-407.
38. Monster, A. C. et al *Int. Arch. Occup. Environ. Health.* 1976, **38**, 87-102.
39. *IPCS Environmental Health Criteria No. 50: Trichloroethylene* 1985, WHO, Geneva, Switzerland.
40. Green, T. et al *Chem. Biol. Interact.* 1997, **105**(2), 99-117.
41. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
42. Verschuere, K. (Ed.) *Handbook of Environmental Data on Organic Chemicals* 1983, Van Nostrand Reinhold, New York, NY, USA.
43. McGregor, D. B. et al *Environ. Mol. Mutagen.* 1989, **13**(3), 197-202.
44. Rossman, T. G. et al *Mutat. Res.* 1991, **260**(4), 349-356.
45. Galloway, S. M. et al *Environ. Mol. Mutagen.* 1987, **10**(Suppl. 10), 1-175.
46. Crebelli, R. et al *Proc. ICMR Semin.* 1981, **8**, 437-442.

47. Nelson, M. A. et al *Toxicol. Appl. Pharmacol.* 1988, **94**(10), 45-54.
48. Nagaya, T. et al *Mutat. Res.* 1989, **222**(3), 279-282.
49. White, R. F. et al *Environ. Res.* 1997, **73**(1-2), 113-124.
50. *Appl. Occup. Environ. Hyg.* 1992, **7**(11), 786-791.
51. *Reprod. Toxicol.* 1996, **10**(4), 295-299.
52. Yoshida, M. et al *Hum. Exp. Toxicol.* 1996, **15**(3), 254-258.
53. Forkert, P. G. et al *Drug Metab. Dispos.* 1989, **17**(1), 106-113.
54. *Gov. Rep. Announce. Index (U.S.)* 1990, **90**(6), Abstr. No. 012,510 (*Chem. Abstr.* **114**, 57300z).
55. Kautiainen, A. et al *Chem.-Biol. Interact.* 1997, **106**(2), 109-121.
56. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
57. *Occupational Exposure Limits: Criteria Document Summaries* 1993, HMSO, London, UK.
58. *Chem. Health Saf.* 1997, **4**(2), 29.
59. Bazin, C. et al *Sci. Eau* 1987, **6**(4), 403-413 (Fr.) (*Chem. Abstr.* **108**, 17344m).
60. *IARC Monograph* 1979, **20**, 545-572.
61. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T250 trichloroisocyanuric acid



$C_3Cl_3N_3O_3$

Mol. Wt. 232.41

CAS Registry No. 87-90-1

Synonyms trichlorocyanuric acid; trichloro-s-triazinetriene; isocyanuric chloride; 1,3,5-trichloro-1,3,5-triazine-2,4,6-(2H,3H,5H)-trione; Queschlor; Oniachlor 90; Master

EINECS No. 201-782-8

RTECS No. XZ 1925000

Uses Disinfectant. In household cleaners.

Physical properties

M. Pt. 246-247°C (decomp.)

Occupational exposure

Supply classification oxidising, harmful

Risk phrases Contact with combustible material may cause fire – Harmful if swallowed – Contact with acids liberates toxic gas – Irritating to eyes and respiratory system (R8, R22, R31, R36/37)

Safety phrases Keep out of reach of children (if sold to general public) – Keep container dry – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – In case of fire and/or explosion do not breathe fumes (S2, S8, S26, S41)

Ecotoxicity

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 0.626 ppm Microtox test (1).

Bioaccumulation

Confirmed to be non or low accumulative (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 406 mg kg⁻¹ (3).

LD₅₀ dermal rabbit 20 g kg⁻¹ (3).

Irritancy

Dermal rabbit (24 hr) 500 mg caused moderate irritation and 50 µg instilled into rabbit eye (24 hr) caused severe irritation (4).

3125 mg instilled into rabbit eye caused moderate irritation (5).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level 1 µg l⁻¹ (6).

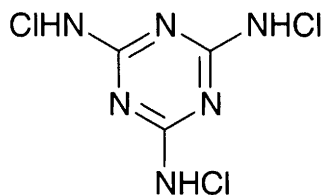
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties, environmental effects listed (7).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
2. *The list of the existing chemical substances tested on biodegradability by microorganisms or bioaccumulation in fish body* 1987, Chemicals Inspection & Testing Institute, Japan.
3. *Toxicol. Appl. Pharmacol.* 1977, **42**, 417.
4. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
5. *Monsanto Co. Toxicity Information* 1972, Monsanto Industrial Chemicals Co., Wilmington, USA.
6. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
7. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T251 trichloromelamine



C₃H₃Cl₃N₆

Mol. Wt. 229.46

CAS Registry No. 7673-09-8

Synonyms *N,N',N''*-trichloro-1,3,5-triazine-2,4,6-triamine; *N*²,*N*⁴,*N*⁶-trichloromelamine

EINECS No. 231-648-4

RTECS No. XZ 1575000

Physical properties

M. Pt. >300°C

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird >100 mg kg⁻¹ (1).

References

1. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382

T252 trichloromethanesulfenyl chloride



CCl₄S

Mol. Wt. 185.89

CAS Registry No. 594-42-3

Synonyms perchloromethyl mercaptan; trichloromethylsulfenyl chloride

EINECS No. 209-840-4

RTECS No. PB 0370000

Physical properties

B. Pt. 146-148°C Specific gravity 1.70

Occupational exposure

FR-VME 0.1 ppm (0.8 mg m⁻³)

US-TWA 0.1 ppm (0.76 mg m⁻³)

UN No. 1670 HAZCHEM Code 2X Conveyance classification toxic substance

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 83 mg kg⁻¹ (1).

LC₅₀ (2 hr) inhalation mouse 296 mg m⁻³ (2).

LD₅₀ intravenous mouse 56 mg kg⁻¹ (3).

Irritancy

Dermal rabbit (24 hr) 500 mg caused severe irritation and 50 µg instilled into rabbit eye (24 hr) caused severe irritation (1).

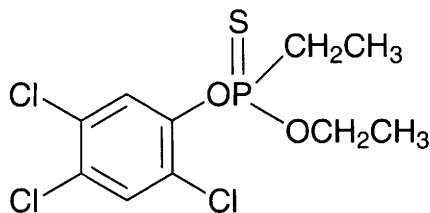
Legislation

Recommended for testing under the US Federal Toxic Substances Control Act (4).

References

1. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
2. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
3. *US Armament Research and Development Command* NX 06768, Chemical Systems Lab., NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD, USA.
4. *Fed. Regist.* 06 Mar 1991, **56**(44), 9534-9572

T253 trichloronate



$C_{10}H_{12}Cl_3O_2PS$

Mol. Wt. 333.60

CAS Registry No. 327-98-0

Synonyms O-ethyl O-(2,4,5-trichlorophenyl) ethylphosphonothioate; BAY 37282; trichloronat; Agrisil; Agritox; Phytosol

EINECS No. 206-326-1

RTECS No. TB 0700000

Uses Superseded insecticide.

Physical properties

B. Pt. 108°C at 0.01 mmHg **Specific gravity** 1.365 at 20°C with respect to water at 4°C

Volatility v.p. 2×10^{-5} mmHg at 20°C

Solubility Water: 50 ppm at 20°C

Occupational exposure

Supply classification very toxic, dangerous for the environment

Risk phrases Toxic in contact with skin – Very toxic if swallowed – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R24, R28, R50/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Do not breathe vapour – After contact with skin, wash immediately with plenty of water – Wear suitable protective clothing and gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S23, S28, S36/37, S45, S60, S61)

Environmental fate

Degradation studies

$t_{1/2}$ of an initial concentration of 10 ppm in sterile sandy loam, sterile organic soil, non-sterile sandy loam and non-sterile organic soil >24, >24, 1.5 and 4 wk, respectively (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird, house sparrow, quail 1.6-4.22, 5.62 and 23.5 mg kg⁻¹, respectively (2).

LD₅₀ oral cat, rat, rabbit, mouse 10-40 mg kg⁻¹ (3-5).

LC_{Lo} (duration unspecified) inhalation rat 700 mg m⁻³ (5).

LD₅₀ dermal rat 64 mg kg⁻¹ (6).

Legislation

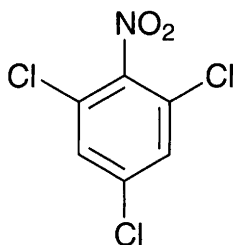
Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (7).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (8).

References

1. Miles, V. R. W. et al *Bull. Environ. Contam. Toxicol.* 1979, **22**, 312-318.
2. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
3. *Wirksubstanzen der Pflanzenschutz und Schaedlingsbekaempfungsmittel* 1976, 71, Verlag Paul Parey, Berlin, Germany.
4. *USDA Information Memorandum* 1966, **20**, 4, Agricultural Research Service, Beltsville, MD, USA.
5. *Pflanzenschutz- und Schaedlingsbekaempfungsmittel: Abriss einer Toxikologie und Therapie von Vergiftungen* 2nd ed., 1971, 35, Hundt-Verlag, Hattingen, Germany.
6. *World Rev. Pest Control* 1970, **9**, 119.
7. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
8. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T254 2,4,6-trichloronitrobenzene



$C_6H_2Cl_3NO_2$

Mol. Wt. 226.45

CAS Registry No. 18708-70-8

Synonyms 1,3,5-trichloro-2-nitrobenzene

EINECS No. 242-518-1

Physical properties

M. Pt. 71°C

Solubility Water: insoluble. Organic solvents: carbon disulfide, ligroin

Ecotoxicity

Invertebrate toxicity

EC₅₀ (5-30 min) *Photobacterium phosphoreum* 0.881 ppm Microtox test (1).

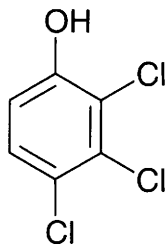
Bioaccumulation

Mean bioconcentration factor in trout over 36 day exposure 760 (2).

References

1. Niimi, A. J. et al *Environ. Toxicol. Chem.* 1989, **8**, 817-823.
2. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431

T255 2,3,4-trichlorophenol



$C_6H_3Cl_3O$

EINECS No. 240-083-2

Mol. Wt. 197.45

CAS Registry No. 15950-66-0

Physical properties

M. Pt. 79-81°C

Occupational exposure

SE-LEVL 0.5 mg m⁻³

SE-STEL 1.5 mg m⁻³

Ecotoxicity

Invertebrate toxicity

Lowest concentration to inhibit growth *Staphylococcus aureus*, *Bacillus subtilis*, *Arthrobacter* sp., *Pseudomonas aeruginosa*, 49.38, 49, 25 and 198 µg ml⁻¹, respectively (1).

EC₅₀ (96 hr) *Selenastrum capricornutum* 2.0 ppm (2).

EC₅₀ (5-30 min) *Photobacterium phosphoreum* 1.25 ppm, Microtox test (3).

Environmental fate

Degradation studies

Not degraded by a pentachlorophenol-degrading *Flavobacterium* which was capable of dechlorinating chlorophenols with chlorine in positions 2 and 6 (4).

Strains of the bacterium *Rhodococcus* (which is found in soil and sludge) degraded 2,3,4-trichlorophenol via hydroxylation to trichlorocatechol, which was then sequentially *O*-methylated to chloroguaiacol and chloroveratrole (5).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird >100 mg kg⁻¹ (6).

Genotoxicity

In vitro Chinese hamster lung cells with and without metabolic activation negative (7).

In vitro Chinese hamster ovary cells without metabolic activation negative, with metabolic activation positive (7).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phenols: maximum admissible concentration 0.5 µg l⁻¹ (8).

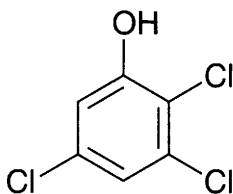
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (9).

References

1. Gotthard, R. et al *Appl. Environ. Microbiol.* 1987, **53**(11), 2689-2692.
2. Shigeoka, T. et al *Environ. Toxicol. Chem.* 1988, **7**, 847-854.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. Steiert, J. G. et al *Appl. Environ. Microbiol.* 1987, **53**(5), 907-910.
5. Haggblom, M. M. et al *Microbiol. Ecol.* 1989, **18**(2), 147-159.
6. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
7. Sofuni, T. et al *Mutat. Res.* 1990, **241**(2), 175-213.
8. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
9. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T256 2,3,5-trichlorophenol



C₆H₃Cl₃O

Mol. Wt. 197.45

CAS Registry No. 933-78-8

EINECS No. 213-272-2

Physical properties

M. Pt. 57-59°C B. Pt. 248-249°C

Occupational exposure

SE-LEVL 0.5 mg m⁻³

SE-STEL 1.5 mg m⁻³

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) guppy 1.6 mg l⁻¹ (1).

Invertebrate toxicity

Lowest concentration to inhibit growth *Staphylococcus aureus*, *Bacillus subtilis*, *Arthrobacter* sp., *Pseudomonas aeruginosa* 49.38, 24.69, 24.69, 395 µg ml⁻¹, respectively (2).

EC₅₀ (5-30 min) *Photobacterium phosphoreum* 1.11 ppm, Microtox test (3).

Environmental fate

Degradation studies

Not degraded by a pentachlorophenol-degrading *Flavobacterium* that was capable of degrading chlorophenols with chlorines at positions 2 and 6 (4).

Degraded by *Rhodococcus* strains; first hydroxylated to trichlorocatechol and then sequentially *O*-methylated to chloroguaiacol and chloroveratrole (5).

Other comments

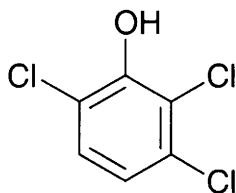
Did not show antibacterial activity against 30 species of bacteria tested (2).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (6).

References

1. Konemann, W. H. *Quantitative structure-activity relationships for kinetics and toxicity of aquatic pollutants in fish* 1979, Univ. Utrecht, Netherlands.
2. Ruckdeschel, G. et al *Appl. Environ. Microbiol.* 1987, 53(11), 2689-2692.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, 26(3), 361-431.
4. Steiert, J. G. et al *Appl. Environ. Microbiol.* 1987, 53(5), 907-910.
5. Haggblom, M. M. *Microbiol. Ecol.* 1989, 18(2), 147-159.
6. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T257 2,3,6-trichlorophenol



C₆H₃Cl₃O

Mol. Wt. 197.45

CAS Registry No. 933-75-5

EINECS No. 213-271-7

RTECS No. SN 1300000

Physical properties

M. Pt. 55-57°C B. Pt. 253°C Flash point 78°C

Occupational exposure

SE-LEVL 0.5 mg m⁻³

SE-STEL 1.5 mg m⁻³

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) guppy 5.1 mg l⁻¹ (1).

Invertebrate toxicity

Lowest concentration to inhibit growth: *Bacillus subtilis*, *Arthrobacter* sp. 395 µg ml⁻¹; *Staphylococcus aureus*, *Pseudomonas aeruginosa* >790 µg m⁻¹ (duration unspecified) (2).

EC₅₀ (5-30 min) *Photobacterium phosphoreum* 12.7 ppm, Microtox test (3).

Bioaccumulation

Leeches in an industrially polluted creek bioaccumulated chlorophenols. The bioconcentration factors for three species were: *Dina dubia* 16500; *Erpobdella punctata* 14000; *Helobdella stagnalis* 7000 (4).

Environmental fate

Degradation studies

A pentachlorophenol-degrading *Flavobacterium* completely dechlorinated 2,3,6-trichlorophenol (5).

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat 308 mg kg⁻¹ (6).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA104 with and without metabolic activation negative (7).

In vitro Chinese hamster lung cells without metabolic activation negative, with metabolic activation positive (8).

In vitro Chinese hamster ovary cells with and without metabolic activation positive (8).

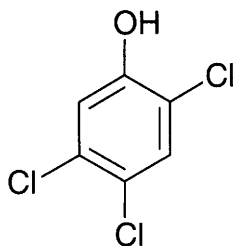
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (9).

References

1. Konemann, W. H. *Quantitative structure-activity relationships for kinetics and toxicity of aquatic pollutants and their mixtures in fish* 1979, Univ. Utrecht, Netherlands.
2. Ruckdeschel, G. et al *Appl. Environ. Microbiol.* 1987, **53**(11), 2689-2692.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. Metcalfe, J. L. et al *Environ. Monit. Assess.* 1988, **11**, 147-169.
5. Steirt, J. G. et al *Appl. Environ. Microbiol.* 1987, **53**(5), 907-910.
6. *Br. J. Pharmacol. Chemother.* 1958, **13**, 20.
7. Strobel, K. et al *Toxicol. Environ. Chem.* 1987, **14**, 143-156.
8. Sofnri, T. et al *Mutat. Res.* 1990, **241**(2), 175-213.
9. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T258 2,4,5-trichlorophenol



C₆H₃Cl₃O

Mol. Wt. 197.45

CAS Registry No. 95-95-4

Synonyms Dowicide 2; Preventol I; TCP (antiseptic)

EINECS No. 202-467-8

RTECS No. SN 1400000

Uses An intermediate in the manufacture of herbicides and pesticides. A rubber additive. An industrial antiseptic.

Physical properties

M. Pt. 67°C B. Pt. 253°C Specific gravity 1.678 at 25°C with respect to water at 4°C

Volatility v.p. 1 mmHg at 72°C

Solubility Water: <0.2 g 100 ml⁻¹. Organic solvents: acetone, benzene, carbon tetrachloride, diethyl ether, methanol, toluene

Occupational exposure

SE-LEVL 0.5 mg m⁻³

SE-STEL 1.5 mg m⁻³

Supply classification harmful, dangerous for the environment

Risk phrases Harmful if swallowed – Irritating to eyes and skin – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R22, R36/38, R50/53)

Safety phrases Keep out of reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – After contact with skin, wash immediately with plenty of water – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S26, S28, S60, S61)

Ecotoxicity

Fish toxicity

Highly cytotoxic to goldfish scale cells cultured *in vitro* (1).

LC₅₀ (96 hr) bluegill sunfish, sheepshead minnow 0.45 and 1.7 mg l⁻¹, respectively (2,3).

LC₅₀ (24 hr) goldfish 1.7 mg l⁻¹ (4).

Invertebrate toxicity

EC₅₀ *Daphnia magna* (24, 48 hr) 1.59 and 0.9 mg l⁻¹ (5).

Lowest concentration to inhibit growth *Arthrobacter* sp. *Staphylococcus aureus*, *Bacillus subtilis*, *Pseudomonas aeruginosa* 24.69, 49.38, 49.38 and 395 µg ml⁻¹, respectively (6).

EC₅₀ (5-30 min) *Photobacterium phosphoreum* 1.27 ppm Microtox test (7).

Bioaccumulation

Fresh water leeches in an industrially polluted creek bioaccumulated chlorophenols; the bioaccumulation factors for 2,4,5-trichlorophenol in three species were: *Dina dubia* 16700; *Erpobdella punctata* 6300; *Helobdella stagnalis* 5700 (8).

Environmental fate

Degradation studies

Mineralised by microorganisms from oligotrophic lakes (9).

Adsorption and retention

Soil sorption coefficient K_{om} 3.36 (10).

Radiolabelled 2,4,5-trichlorophenol was bound to artificial humic acid in the presence of a microbiological soil population; most of the radiolabel remained bound to the humic acid. This suggests that chlorophenols are bound to humus and are released slowly, and so present little environmental threat (11).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 600 and 820 mg kg⁻¹, respectively (12,13).

LD₅₀ intraperitoneal rat 355 mg kg⁻¹ (14).

LD₅₀ subcutaneous rat 2260 mg kg⁻¹ (15).

LD₅₀ intravenous mouse 56 mg kg⁻¹ (16).

Sub-acute and sub-chronic data

Oral (98 day) rat 0.3 or 1 g kg⁻¹ day⁻¹ reduced weight-gain and caused dose-related diuresis, mild centrilobular changes in the liver, moderate degenerative changes in the convoluted tubules of the kidney and early proliferative changes in kidney interstitial tissue (17).

Carcinogenicity and chronic effects

No adequate data for carcinogenicity to humans, limited evidence for carcinogenicity to animals, IARC classification group 3 (18,19).

Sensitisation

In vivo and *in situ* marine local lymph node assay positive. The effect was augmented by pre-exposure for 5 days prior to testing (20).

Genotoxicity

Salmonella typhimurium TA98, TA98, TA100, TA104 with and without metabolic activation negative (21).

In vivo human lymphocytes sister chromatid exchanges and chromosomal aberrations negative (22).

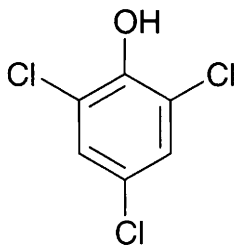
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (23).

References

1. Saito, H. et al *Environ. Toxicol. Chem.* 1991, **10**(2), 235-241.
2. Buccafusco, R. J. et al *Bull. Environ. Contam. Toxicol.* 1981, **26**, 446.
3. Heitmüller, P. T. et al *Bull. Environ. Contam. Toxicol.* 1981, **27**, 596-604.
4. Kobayashi, K. *Am. Chem. Soc. Symp. Ser.* 99 1979.
5. Kuehn, R. et al *Water Res.* 1989, **23**(4), 495-499.
6. Ruckdeschel, G. et al *Appl. Environ. Microbiol.* 1987, **53**, 2689-2692.
7. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
8. Metcalfe, J. L. et al *Environ. Monit. Assess.* 1988, **11**, 147-169.
9. Tranvik, L. et al *Environ. Toxicol. Chem.* 1991, **10**(2), 195-200.
10. Sabljic, A. *QSAR Environ. Toxicol. Proc. Int. Workshop, 2nd 1986 Publ.* 1987, 309-332, Kaiser, K. L. E. (Ed.) Reidel, Dordrecht, Netherlands.
11. Dec, J. et al *Soil Sci. Soc. Am. J.* 1988, **52**(5), 1366-1371.
12. *Pharmazie* 1975, **30** 147.
13. Deichmann *Fed. Proc.* 1943, **2**, 76.
14. *Br. J. Pharmacol. Chemother.* 1958, **13**, 20.
15. *Fed. Proc.* 1943, **2**, 76.
16. *Report NX 03492* US Army Armament Research and Development Command, Chemical Systems Laboratory, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD, USA.
17. McCollister, D. D. et al *Toxicol. Appl. Pharmacol.* 1961, **3**, 63-70.
18. *IARC Monograph* 1987, **Suppl. 7**, 154-156.
19. *IARC Monograph* 1979, **20**, 349-367.
20. Imber, I. et al *J. Appl. Toxicol.* 1991, **11**(2), 129-133.
21. Strobel, K. et al *Toxicol. Environ. Chem.* 1987, **14**(1-2), 143-156.
22. Blank, C. E. et al *Br. J. Ind. Med.* 1983, **40**, 87-91.
23. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T259 2,4,6-trichlorophenol



$C_6H_3Cl_3O$

Mol. Wt. 197.45

CAS Registry No. 88-06-2

Synonyms Dowicide 2S; Omal; Phenachlor

EINECS No. 201-795-9

RTECS No. SN 1575000

Uses Preservative. Fungicide. Bactericide.

Physical properties

M. Pt. 69°C B. Pt. 246°C Flash point none Specific gravity 1.490 at 75°C Volatility v.p. 1 mmHg at 76.5°C

Solubility Water: <0.1 g 100 g⁻¹. Organic solvents: acetone, benzene, carbon tetrachloride, diethyl ether, methanol, toluene

Occupational exposure

SE-LEVL 0.5 mg m⁻³

SE-STEL 1.5 mg m⁻³

Supply classification harmful, dangerous for the environment

Risk phrases Harmful if swallowed – Irritating to eyes and skin – Possible risk of irreversible effects – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R22, R36/38, R40, R50/53)

Safety phrases Keep out of reach of children (if sold to general public) – Wear suitable protective clothing and gloves – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S36/37, S60, S61)

Ecotoxicity

Fish toxicity

In vitro goldfish scale cells, it was less toxic than 2,4,5- and 2,3,4-trichlorophenols (1).

In vitro bluegill sunfish BF-2 cells it was less toxic than 2,3,5-trichlorophenol (2).

Rainbow trout 5 or 50 µg increased the activity of UDP-glucuronyl transferase activity (3).

LC₅₀ (48 hr) killifish 2.3 mg l⁻¹ (4).

LC₅₀ (96 hr) American flagfish 2.26 mg l⁻¹ (5).

Invertebrate toxicity

EC₅₀ *Daphnia magna* (24, 48 hr) 3.7, 2.2 mg l⁻¹, respectively (6).

LC₅₀ (48 hr) juvenile grass shrimp 5.6 mg l⁻¹ (4).

Short-term exposure to (unspecified) sublethal concentrations affected reproduction but not growth of earthworms (7).

EC₅₀ (5-30 min) *Photobacterium phosphoreum* 768 ppm Microtox test (8).

Bioaccumulation

Rainbow trout exposed for 20 days to 5 or 50 µg l⁻¹ accumulated 2,4,6-trichlorophenol in the liver. After 20 days, levels decreased as the fish eliminated the compound (3).

Duck mussels exposed to 6-56 µg l⁻¹ at 3-18°C had a bioconcentration factor of 14,125 (9).

Environmental fate

Degradation studies

26 of 170 soil samples collected from various environments were capable of degrading 2,4,6-trichlorophenol. At concentrations <500 ppm it was completely degraded in 8 days and Cl⁻ was detected in the culture medium; no intermediate product was detected (10).

[¹⁴C]-2,4,6-trichlorophenol applied to soil at 1.78 µg g⁻¹ dry weight soil was incubated under outdoor conditions for 25 wk. After this time 50.4% remained in the soil, radiolabel was found in unchanged parent compound, 2,4,6-trichloroanisole, 2,4,6-trichlorophenyl ethyl ether and unidentified products (11).

Adsorption and retention

Soil sorption coefficient log K_{om} 3.02 (12).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 820 mg kg⁻¹ (13).

LD₅₀ intraperitoneal rat 276 mg kg⁻¹ (14).

Carcinogenicity and chronic effects

Limited evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification 2B (15).

Oral (106-107 wk) Fisher 344 rats 5000 or 10,000 ppm in feed. There was a significant dose-related increase in lymphomas and leukaemias in ♂ rats but not in ♀ (16).

Oral (105 wk) ♂ B6C3F1 mice 5000 or 10,000 ppm in feed, ♀ B6C3F1 mice initially 10,000 or 20,000 ppm in feed (for 38 wk) after which 2500 or 5000 ppm in feed (for a further 67 wk), this gave a time weighted average of 5214 or 10,428 ppm. There was a statistically significant dose-related increased incidence of hepatocellular carcinomas or adenomas (16).

Mouse (78 wk) gavage for 4 wk 100 mg kg⁻¹, oral 260 mg kg⁻¹ in feed until 78 wk. When ♂ and ♀ findings were taken together there was a statistically significant increase in the incidence of hepatoma and reticulum-cell sarcomas. These incidences were not significant when ♂ and ♀ results were analysed separately (17).

Metabolism and toxicokinetics

Following *in vitro* incubation with rat liver 3-9 fraction, three metabolites were identified 2,6-dichloro-1,4-hydroquinone; and two isomers of hydroxypentachlorodiphenyl ether (18).

In humans occupationally exposed over a season of timber treatment, maximum urinary concentrations were 0.20-2.33 µg l⁻¹. The apparent t_{1/2} was 18 hr, calculated using a 1-compartment model (19).

Irritancy

Dermal (24 hr) rabbit 500 mg kg⁻¹ caused moderate irritation, 50 µg instilled into rabbit eye caused severe irritation (20).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA104 with and without metabolic activation negative (21).

In vitro Chinese hamster ovary cells with and without metabolic activation sister chromatid exchanges, chromosomal aberrations negative (22).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (23).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (24).

Other comments

Carcinogenicity reviewed (25).

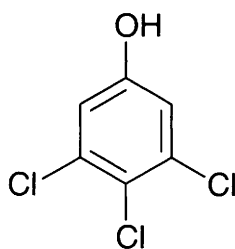
Toxicity reviewed (26).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (27).

References

1. Saito, H. et al *Environ. Toxicol. Chem.* 1991, **10**(2), 235-241.
2. Bubich, H. et al *Environ. Res.* 1987, **42**(1), 229-237.
3. Tana, J. J. *Water Sci. Technol.* 1988, **20**(2), 77-85.
4. Burton, D. T. et al *Environ. Contam. Toxicol.* 1990, **44**(5), 776-783.
5. Smith, A. D. et al *Arch. Environ. Contam. Toxicol.* 1991, **20**, 94-102.
6. Keuehn, R. et al *Water Res.* 1989, **23**(4), 495-499.
7. Neuhauser, E. F. et al *Soil Biol. Biochem.* 1990, **22**(2), 175-179.
8. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
9. Makela, T. P. et al *Ecotoxicol. Environ. Saf.* 1991, **22**(2), 175-179.
10. Kiyohara, H. et al *J. Ferment. Bioeng.* 1989, **67**(5), 339-344.
11. Schmitzer, J. et al *Chemosphere* 1989, **18**(11-12), 2383-2388.
12. Sabljic, A. *QSAR Environ. Toxicol. Proc. Int. Workshop, 2nd 1986 Publ.* 1988, 309-302, Kaiser, K. L. E. (Ed.), Reidel, Dordrecht, Netherlands.
13. *Pesticide Chemicals Official Compendium* 1966, 1176, Association of the American Pesticide Control Officials Inc., Topeka, KS, USA.
14. *Br. J. Pharmacol. Chemother.* 1958, **13**, 20.
15. *IARC Monograph* 1987, **Suppl. 7**, 154-156.
16. *NTIS Report* 155, Natl. Tech. Inf. Ser., Springfield, VA, USA.
17. Innes, J. R. M. et al *J. Natl. Cancer Inst.* 1969, **42**, 1101-1114.
18. Juhl, U. et al *Chem.-Biol. Interact.* 1989, **69**(4), 333-344.
19. Pekari, K. et al *Int. Arch. Occup. Environ. Health* 1991, **63**(1), 57-62.
20. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vyetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
21. Strobel, K. et al *Toxicol. Environ. Chem.* 1987, **14**(1-2), 143-156.
22. Galloway, S. M. et al *Environ. Mol. Mutagen.* 1987, **10**(Suppl. 10), 1-175.
23. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
24. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
25. *Comm. Eur. Communities [Rep.] EUR* 1990, EUR 12481, *Toxicol. Chem.*, 1: Carcinog., Vol. 12, 121-125.
26. *BIBRA Toxicity Profile* 1991, British Industrial Biological Research Association, Carshalton, UK.
27. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T260 3,4,5-trichlorophenol



$C_6H_3Cl_3O$

Mol. Wt. 197.45

CAS Registry No. 5609-19-8

Physical properties

B. Pt. 185-186°C at 1 mmHg Specific gravity 0.9759 at 20°C

Occupational exposure

SE-LEVL 0.5 mg m⁻³

SE-STEL 1.5 mg m⁻³

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) guppy 1.1 mg l⁻¹ (1).

Invertebrate toxicity

Lowest concentration (5 day) to inhibit growth: *Staphylococcus aureus*, *Bacillus subtilis*, *Arthrobacter* sp. 12.25 µg ml⁻¹; *Pseudomonas aeruginosa* 98.75 µg ml⁻¹ (2).

EC₅₀ (5-30 min) *Photobacterium phosphoreum* 0.359 ppm Microtox test (3).

Environmental fate

Degradation studies

Degraded in an anaerobic upflow bioreactor, with major microorganisms being *Methanosarcina* and *Methanothrix* and a putative anaerobic phenol-oxidising bacterium (4).

A pentachlorophenol-degrading *Flavobacterium* could not significantly degrade 3,4,5-trichlorophenol; phenols with chlorine at positions 2 and 6 were significantly dechlorinated (5).

Rhodococcus strains found in soil and sludge degraded 3,4,5-trichlorophenol, first via hydroxylation to trichlorocatechol and then sequentially *O*-methylated to chloroguaiacol to chloroveratrole (6).

Adsorption and retention

Soil sorption. coefficient log K_{om} 3.56 (7).

Genotoxicity

In vitro Chinese hamster lung cells without metabolic action negative, with metabolic activation equivocal (8).

In vitro Chinese hamster ovary cells with and without metabolic activation negative (8).

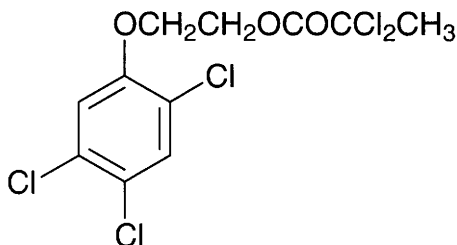
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (9).

References

1. Konemann, W. H. *Quantitative structure-activity relationship for kinetics and toxicology of aquatic pollutants and their mixtures in fish* 1979, Univ. Utrecht, Netherlands.
2. Ruckdeschel, G. et al *Appl. Environ. Microbiol.* 1987, **53**(11), 2689-2692.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. Krumme, M. L. et al *Water Res.* 1988, **22**(2), 171-177.
5. Steiert, J. G. et al *Appl. Environ. Microbiol.* 1987, **53**(5), 907-910.
6. Haggblom, M. M. *Microb. Ecol.* 1989, **18**(2), 147-159.
7. Sabljic, A. *QSAR Environ. Toxicol. Proc. Int. Workshop, 2nd 1986 Publ.* 1987, 309-332, Kaiser K. L. E. (Ed.), Reidel, Dordrecht, Netherlands.
8. Sofuni, T. et al *Mutat. Res.* 1990, **241**(2), 175-213.
9. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T261 2-(2,4,5-trichlorophenoxy)ethyl 2,2-dichloropropionate



$C_{11}H_9Cl_5O_3$

Mol. Wt. 366.45

CAS Registry No. 136-25-4

Synonyms propanoic acid, 2,2-dichloro-, 2-(2,4,5-trichlorophenoxy)ethyl ester; propionic acid, 2,2-dichloro-, 2-(2,4,5-trichlorophenoxy)ethyl ester; Baron; erbon; Novon; Pentanate

RTECS No. UF 1400000

Uses Superseded herbicide.

Physical properties

M. Pt. 49-50°C **B. Pt.** 161-164°C at 0.5 mmHg **Specific gravity** 1.55 at 50°C with respect to water at 4°C
Solubility Organic solvents: acetone, ethanol, kerosene, xylene

Occupational exposure

Supply classification harmful, dangerous for the environment

Risk phrases Harmful if swallowed – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R22, R51/53)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S61)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1000 mg kg⁻¹ (1).

LD₅₀ oral mouse, rabbit 912, 2193 mg kg⁻¹, respectively (2).

Other effects

Other adverse effects (human)

No causal association could be found between the long-time exposure of workers engaged in the manufacture of the compound and their mortality rates from malignant neoplasms (cancers of the stomach, liver, connective tissue, lymphomas, and nasopharyngeal system). A statistically significant association was obtained between exposure and mortality from cirrhosis of the liver, but this could be due to alcohol abuse (3).

Legislation

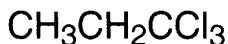
Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (4).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (5).

References

1. *Farm Chemicals Handbook* 1980, Meister Publishing, Willoughby, OH, USA.
2. *Hyg. Sanit.* 1969, **34**, 174.
3. Ott, M. et al *J. Occup. Med.* 1987, **29**(5), 422-429.
4. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
5. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T262 1,1,1-trichloropropane



$\text{C}_3\text{H}_5\text{Cl}_3$

Mol. Wt. 147.43

CAS Registry No. 7789-89-1

RTECS No. TZ 8750000

Physical properties

B. Pt. 140°C

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 7460 mg kg⁻¹ (1).

LC_{Lo} (4 hr) inhalation rat 8000 ppm (1).

Irritancy

Dermal rabbit (24 hr) 10 mg caused mild irritation and 20 mg instilled into rabbit eye caused severe irritation (2).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level 1 µg l⁻¹ (3).

References

1. *Am. Ind. Hyg. Assoc. J.* 1962, **23**, 95.
2. *AMA Arch. Ind. Hyg. Occup. Med.* 1954, **10**, 61.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T263 1,1,2-trichloropropane



$\text{C}_3\text{H}_5\text{Cl}_3$

Mol. Wt. 147.43

CAS Registry No. 598-77-6

EINECS No. 209-951-8

RTECS No. TZ 8925000

Mammalian & avian toxicity

Acute data

LC₅₀ (4 hr) inhalation rat 2000 ppm (1).

LD₅₀ dermal rabbit 14,100 mg kg⁻¹ (1).

Irritancy

Dermal rabbit (24 hr) 10 mg caused mild irritation and 20 mg instilled in a rabbit eye caused severe irritation (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level 1 µg l⁻¹ (2).

References

1. *AMA Arch. Ind. Hyg. Occup. Med.* 1954, **10**, 61.
2. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T264 1,2,3-trichloropropane



$\text{C}_3\text{H}_5\text{Cl}_3$

Mol. Wt. 147.43

CAS Registry No. 96-18-4

Synonyms glycerol trichlorohydrin; trichlorohydrin; allyl trichloride

EINECS No. 202-486-1

RTECS No. TZ 9275000

Uses Paint and varnish remover. Degreasing agent. Cross-linking agent.

Physical properties

M. Pt. -14°C B. Pt. 156°C Flash point 82°C Specific gravity 1.417 at 15°C with respect to water at 4°C

Volatility v.p. 2 mmHg at 20°C; v.den. 5.08

Occupational exposure

UK-LTEL 50 ppm (306 mg m⁻³)

UK-STEL 75 ppm (460 mg m⁻³)

US-TWA 10 ppm (60 mg m⁻³)

Supply classification harmful

Risk phrases Harmful by inhalation, in contact with skin and if swallowed (R20/21/22)

Safety phrases Keep out of reach of children (if sold to general public) – Wear suitable gloves and eye/face protection (S2, S37/39)

Ecotoxicity

Fish toxicity

LC₅₀ (7 day) guppy 42 mg l⁻¹ (1).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 24.5 ppm Microtox test (2).

Environmental fate

Nitrification inhibition

IC₅₀ (25 day) *Nitrosomonas* 30 mg l⁻¹ (3).

Anaerobic effects

IC₅₀ (50 day) methanogenic bacterial culture 0.63 mg l⁻¹ (3).

Degradation studies

Soil t_{1/2} 2-7 days (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 320 mg kg⁻¹ (5).

LD_{Lo} oral dog 200 mg kg⁻¹ (6).

LC₅₀ (2 hr) inhalation mouse 3400 mg m⁻³ (7).

LC_{Lo} (4 hr) inhalation rat 1000 ppm (8).

LD₅₀ dermal rabbit 1770 mg kg⁻¹ (8).

Sub-acute and sub-chronic data

Gavage rats (17 wk) 8, 16, 32, 63, 125 or 250 mg kg⁻¹ in corn oil 5 day wk⁻¹. All rats receiving 250 mg kg⁻¹ died by wk 5; 1 ♂ and 4 ♀ receiving 125 mg kg⁻¹ died during the study. Final mean body weights of ♂ given 63 mg kg⁻¹ and ♂ and ♀ given 125 mg kg⁻¹ were lower than those of controls. Haemocrit values, haemoglobin concentrations and erythrocyte counts decreased with dose in all treated animals; serum pseudocholinesterase activity also decreased with dose in ♀. Serum alanine aminotransferase, aspartate aminotransferase and sorbitol dehydrogenase activities were increased in ♀s receiving 125 mg kg⁻¹. The principal toxic lesions were hepatocellular necrosis, karyomegaly and biliary hyperplasia of the liver; renal tubule necrosis, regeneration and karyomegaly of the kidney; and necrosis and inflammation of the nasal olfactory and respiratory epithelium (9). Gavage mice (17 wk) 8, 16, 32, 63, 125 or 250 mg kg⁻¹ body weight in corn oil 5 days wk⁻¹. 16/20 ♂ and 7/20 ♀ mice given 250 mg kg⁻¹ died by wk 4. Only the body weights of ♂s given 250 mg kg⁻¹ were lower than those of controls. The principal toxic lesions were hepatocellular necrosis and karyomegaly of the liver; necrosis, regeneration, and hyperplasia of the bronchiolar epithelium in the lung; and acanthosis (hyperplasia) and hyperkeratosis of the forestomach epithelium (9).

Carcinogenicity and chronic effects

National Toxicology Program tested rats and mice via gavage. Clear evidence of carcinogenicity (increased incidence of dose-related malignant and benign neoplasms) in ♂, ♀ rats and mice (9).

National Toxicology Program classification: reasonably anticipated to be a human carcinogen (10).

Gavage rat (2 yr) 0, 3, 10 or 30 mg kg⁻¹ body weight in corn oil 5 days wk⁻¹. Survival of both ♂ and ♀ rats receiving 10 or 30 mg kg⁻¹ was reduced compared with that of controls. Final mean body weights of rats given 30 mg kg⁻¹ were lower than controls, while weights of other animals were similar to controls. Benign and malignant neoplasms of the oral mucosa, forestomach, and preputial and clitoral glands in ♂s and ♀s, benign neoplasms of the exocrine pancreas and kidney in ♂s, and malignant neoplasms of the mammary glands in ♀s were observed (9).

Gavage mice (2 yr) 0, 6, 20 or 60 mg kg⁻¹ body weight in corn oil 5 days wk⁻¹. Survival of all treated animals was lower than controls. Final mean body weights of ♂ receiving 20 or 60 mg kg⁻¹ and ♀ receiving 60 mg kg⁻¹ were lower than those of controls. Squamous cell papillomas and carcinomas of the forestomach were seen in all treated mice. The incidences of squamous cell carcinomas of the oral mucosa, uterine adenoma, adenocarcinoma, stromal polyp and hepatocellular adenoma or carcinoma were increased in ♀s receiving 60 mg kg⁻¹. The

incidences of hepatocellular adenoma or carcinoma were also increased in all dosed ♂s. Harderian gland adenoma were increased in ♂s given 20 or 60 mg kg⁻¹ and ♀s given 60 mg kg⁻¹ (9).

Teratogenicity and reproductive effects

♀ and ♂ rats were administered the compound by gavage (dose and duration unspecified). At higher doses few pairs delivered 3, 4 or 5 litters and the litters had fewer pups. Parental body weights were not decreased but ♀ kidney and ovary weights, and epididymal weights were reduced; liver weights were increased. Sperm parameters were unchanged (11).

Inhalation ♂, ♀ rats 0-900 ppm 6 hr day⁻¹, 5 day wk⁻¹ for up to 4 wk. Ovary weights of ♀ exposed to 300 or 600 ppm and spleen weights of ♀ exposed to 300 ppm were lower than controls. ♂ exposed to 600 ppm had decreased testes weights. Liver weights of animals exposed to ≤600 ppm were increased and body weight of all treated animals were decreased compared with controls. 9/10 animals died after a single exposure to 900 ppm; 1/10 and 3/10 animals died after exposure to 300 and 600 ppm, respectively (12).

Irritancy

Dermal rabbit 700 mg caused mild irritation and 140 mg instilled in a rabbit eye caused severe irritation (durations unspecified) (5).

Genotoxicity

Salmonella typhimurium TA100, TA153K with metabolic activation positive (13).

Salmonella typhimurium TA97, TA98, TA100, TA1535 with metabolic activation positive; TA1537 with and without metabolic activation negative (9).

Escherichia coli P437 SOS chromotest with and without metabolic activation negative (14).

In vitro mouse lymphoma L5178Y with metabolic activation positive (9).

In vitro Chinese hamster ovary cells with metabolic activation sister chromatid exchanges, chromosomal aberrations positive (9).

Induced hepatic DNA damage (strand breaks) in rats as rapidly as 1 hr after an intraperitoneal dose (15).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level 1 µg l⁻¹ (16).

Other comments

An impurity in some nematocides and soil fumigants. A contaminant of drinking and ground water (9).

Reviews on human health effects, experimental toxicology, physico-chemical properties, epidemiology, workplace experience, exposure levels, environmental effects, ecotoxicology listed (17).

References

1. Koenemann, W. H. *Quantitative structure-activity relationships for kinetics and toxicity of aquatic pollutants and their mixtures in fish* 1979, Univ. Utrecht, Netherlands.
2. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
3. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, **63**(3), 198-207.
4. Anderson, T. A. et al *J. Environ. Qual.* 1991, **20**(2), 420-424.
5. *Union Carbide Data Sheet* 20th March 1973.
6. *Am. J. Hyg.* 1932, **16**, 325.
7. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
8. *Am. Ind. Hyg. Assoc. J.* 1962, **23**, 95.
9. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-384, NIEHS, Research Triangle Park, NC, USA.
10. *Eighth Report on Carcinogens* 1998, National Toxicology Program, NIEHS, Research Triangle Park, NC 27709, USA.
11. Gulati, D. K. et al *Report* 1990, NTP-90-209, Order No. PB91-129676.
12. Johannsen, F. R. et al *J. Toxicol. Environ. Health* 1988, **25**(3), 299-315.
13. Rapton, F. et al *Environ. Mol. Mutagen.* 1988, **12**(2), 253-259.

14. Von der Hude, W. et al *Mutat. Res.* 1988, **203**, 81-94.
15. Weber, G. L. et al *Adv. Exp. Med. Biol.* 1991, **283**(Biol. React. Intermed. 4), 853-855.
16. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
17. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T265 1,2,3-trichloro-1-propene



$\text{C}_3\text{H}_3\text{Cl}_3$

Mol. Wt. 145.41

CAS Registry No. 96-19-5

Synonyms 2,3-dichloroallyl chloride

EINECS No. 202-487-7

RTECS No. UD 2450000

Physical properties

B. Pt. 142°C

Environmental fate

Abiotic removal

Evaporation from water at 25°C at 1 ppm: 50% after 49 min; 90% after >140 min (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 616 mg kg⁻¹ (2).

LC_{Lo} (4 hr) inhalation rat 500 ppm (2).

LD_{Lo} skin rabbit 640 mg kg⁻¹ (3).

Sub-acute and sub-chronic data

Inhalation rat (13 wk) 0, 1, 5 or 15 ppm 6 hr day⁻¹, 5 day wk⁻¹. Signs of nasal irritation were seen in animals exposed to 15 ppm, but no other effects considered to be related to treatment were observed (4).

Oral rat (4 wk) 0-300 mg kg⁻¹ day⁻¹. All rats given 300 mg kg⁻¹ died, and mean body weights were reduced in ♂ rats given 100 mg kg⁻¹ (5).

Teratogenicity and reproductive effects

Inhalation rat 0, 1 or 5 ppm 6 hr day⁻¹, 5 day wk⁻¹ for a 10-wk premating period, the mating period, and the first 14 days of gestation (♀ only). No effects were seen on pup survival, sex distribution, body weights or organ weights. No treatment-related effects were seen following necropsy of adults or weanlings or following microscopic evaluation of gonads from parental animals (4).

Irritancy

Dermal rabbit (24 hr) 10 mg caused severe irritation (3).

50 mg instilled into rabbit eye caused moderate irritation (duration unspecified) (2).

Genotoxicity

Salmonella typhimurium TA98, TA100 with and without metabolic activation positive (6).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level 1 $\mu\text{g l}^{-1}$ (7).

References

1. Wendell, L. D. et al *Environ. Sci. Tech.* 1975, **9**(9).
2. *Union Carbide Data Sheet* 4th May 1960.
3. *Am. Ind. Hyg. Assoc. J.* 1962, **23**, 95.
4. Johannsen, F. R. et al *J. Toxicol. Environ. Health* 1991, **33**(3), 291-302.
5. Johannsen, F. R. et al *Toxicol. Lett.* 1991, **57**(3), 347-352.
6. Matsuda, H. et al *Sci. Total Environ.* 1991, **103**, 141-149.
7. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T266 3,3,3-trichloro-1-propene



$\text{C}_3\text{H}_3\text{Cl}_3$

Mol. Wt. 145.41

CAS Registry No. 2233-00-3

Synonyms RTECS No. UD 1928700

Physical properties

M. Pt. -30°C B. Pt. $114\text{--}115^\circ\text{C}$ Specific gravity 1.3296 at 50°C
Solubility Organic solvents: benzene, chloroform, diethyl ether, ethanol

Genotoxicity

In vivo mouse liver cells increased the percentage of unwound DNA at 300 mg kg^{-1} for 4 hr (1).
In vivo mouse bone marrow cells sister chromatid exchanges negative (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level 1 $\mu\text{g l}^{-1}$ (2).

References

1. Giri, A. K. et al *Mutat. Res.* 1990, **242**, 187-194.
2. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T267 trichlorosilane



Cl_3HSi

Mol. Wt. 135.45

CAS Registry No. 10025-78-2

Synonyms silicochloroform; silicon chloride hydride

EINECS No. 233-042-5

RTECS No. VV 5950000

Physical properties

M. Pt. -126.5°C B. Pt. 31.8°C Flash point -13°C Specific gravity 1.35 at 0°C Volatility v.p. 40 mmHg at 14.5°C ; v.den. 4.7

Solubility Water: decomposes. Organic solvents: benzene, chloroform, carbon disulfide, carbon tetrachloride

Occupational exposure

UN No. 1295 HAZCHEM Code 4WE Conveyance classification substance which in contact with water emits flammable gas, danger of fire (flammable liquid), corrosive

Supply classification highly flammable

Risk phrases Contact with water liberates extremely flammable gases – Spontaneously flammable in air (R15, R17)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with skin and eyes – In case of fire, use alcohol foam dry chemical or carbon dioxide – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S2, S24/25, S43, S45)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1030 mg kg⁻¹ (1).

LC₅₀ (2 hr) inhalation mouse 1500 mg m⁻³ (2).

LC_{Lo} (4 hr) inhalation rat 1000 ppm (3).

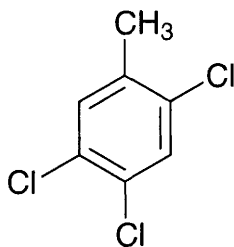
Other comments

Reviews on human health effects, experimental toxicology, environmental effects, ecotoxicology, exposure levels, physico-chemical properties listed (4).

References

1. *J. Ind. Hyg. Toxicol.* 1949, **31**, 60.
2. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
3. *J. Ind. Hyg. Toxicol.* 1949, **31**, 343.
4. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T268 2,4,5-trichlorotoluene



$C_7H_5Cl_3$

Mol. Wt. 195.47

CAS Registry No. 6639-30-1

Synonyms 1,2,4-trichloro-5-methylbenzene

EINECS No. 229-644-2

Physical properties

M. Pt. -80 – $-83^{\circ}C$ B. Pt. 229 – $230^{\circ}C$ at 716 mmHg Partition coefficient $\log P_{ow}$ 4.72 (1)

Solubility Organic solvents: acetone, ethanol

Ecotoxicity

Fish toxicity

LC_{50} (7 day) guppy 1.7 mg l^{-1} (2).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level $1\text{ }\mu\text{g l}^{-1}$ (3).

The $\log P_{ow}$ value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (4).

References

1. Abernethy, S. G. et al *Environ. Toxicol. Chem.* 1988, 7, 469-481.
2. Koenemann, W. H. *Quantitative structure activity relationships for kinetics and toxicity of aquatic pollutants and their mixtures in fish* 1979, Univ. Utrecht, Netherlands.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
4. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; 6th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK

T269 1,1,2-trichlorotrifluoroethane



$C_2Cl_3F_3$

Mol. Wt. 187.38

CAS Registry No. 76-13-1

Synonyms 1,1,2-trichloro-1,2,2-trifluoroethane; 1,2,2-trichlorotrifluoroethane; Freon 113; Freon TF; Frigen 113; R 113; Arcton 63; Daiflon S3; Genetron 113; CFC-113

EINECS No. 200-936-1

RTECS No. KJ 4000000

Uses In refrigerants, propellants, solvents and fire extinguishing agents. Also used in dry-cleaning operations.

Physical properties

M. Pt. -35°C B. Pt. 47-48°C Flash point none Specific gravity 1.56 at 25°C
Partition coefficient $\log P_{ow}$ 3.16 (1) Volatility v.p. 360 mmHg at 20°C; v.den. 6.47
Solubility Water: 100 mg l⁻¹ at 20°C. Organic solvents: benzene, diethyl ether, ethanol

Occupational exposure

DE-MAK 500 ppm (3900 mg m ⁻³)	FR-VLE 1250 ppm (9500 mg m ⁻³)
FR-VME 1000 ppm (7600 mg m ⁻³)	
JP-OEL 500 ppm (3800 mg m ⁻³)	SE-STEL 750 ppm (6000 mg m ⁻³)
SE-LEVL 500 ppm (4000 mg m ⁻³)	UK-STEL 1250 ppm (9740 mg m ⁻³)
UK-LTEL 1000 ppm (7790 mg m ⁻³)	US-STEL 1250 ppm (9590 mg m ⁻³)
US-TWA 1000 ppm (7670 mg m ⁻³)	

Ecotoxicity

Bioaccumulation

Bioconcentration factors of 34 and 11 have been estimated, based on water solubility and the P_{ow} value, respectively. These values suggest the compound would not bioaccumulate significantly in aquatic organisms (2).

Environmental fate

Anaerobic effects

IC₅₀ (50 day) methanogenic bacterial culture 3.7 mg l⁻¹ (3).

Abiotic removal

If released into soil, the compound would rapidly volatilise from the surface or leach through the soil into ground water. If released into water, all of the compound would be lost by volatilisation ($t_{1/2}$ 4 hr from a model river). If released into the atmosphere, all of the compound would exist in the vapour phase. Not degraded in the troposphere and so diffusion from the troposphere to the stratosphere would be the sole removal mechanism ($t_{1/2}$ 20 yr). Direct photolysis is the dominant removal mechanism in the stratosphere ($t_{1/2}$ 63-122 yr) (2).

Adsorption and retention

Soil adsorption coefficients of 191 and 259 have been estimated using linear regression equations based on the P_{ow} and water solubility, respectively. These values suggest the compound would be moderately mobile in soil and that moderate adsorption to suspended solids and sediments in water would take place (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 45 mg kg⁻¹ (4).
LC_{Lo} (6 hr) inhalation rat 87,000 ppm (5).
LC_{Lo} (90 sec) inhalation mouse 25 pph (6).

Carcinogenicity and chronic effects

Inhalation rat (1 yr) 6 hr day⁻¹ 5 days wk⁻¹; average exposure concentrations were 0, 2000, 10,000 and 20,000 ppm. Body weights were lower in ♂ and ♀ rats exposed to 20,000 ppm after 1 and 4 months, respectively, and in ♀ rats exposed to 10,000 ppm after 1 yr. Microscopic examination of tissues revealed no evidence of compound-related toxicity or carcinogenicity. The no-observable-adverse-effect level for this study was 2000 ppm (7).

Irritancy

Dermal rabbit 500 mg caused mild irritation (duration unspecified) (8).
Not irritating to rabbit eye (9).
Removes fats and oils from the skin and produces skin dryness; however, there is little skin absorption (9).

Genotoxicity

Predicted to be highly genotoxic following a quantitative structure-activity relationship (QSAR) study (10).

Other effects

Other adverse effects (human)

The principal effects of chlorofluorocarbon toxicity in humans from inhalation include respiratory distress, cardiotoxicity, severe arrhythmias, bronchopneumonia, and asthma. Acute inhalation exposure causes dizziness, narcosis and hallucinations; repeated inhalation does not produce liver toxicity. Chlorofluorocarbons have also been implicated in adverse effects to the bronchopulmonary system, including bronchospasms (9).

Loss of ability to concentrate and mild lethargy is seen in humans exposed to 2500 ppm (11).

Increased numbers and unexplained deaths from bronchial asthma have been attributed to cardiotoxicity from bronchodilator aerosol propellants (12).

No symptoms of adverse effects were seen in workers exposed to 46-4700 ppm for ~3 yr (13).

Any other adverse effects

Inhalation studies in animals have confirmed that the compound produces weak narcosis and cardiotoxicity, with irritation of the respiratory tract and sleepiness at 12,000 ppm (9).

Liver microsomal extracts from mice given single intraperitoneal injections of the compounds showed significant increases in their ability to activate carcinogenic polyaromatic hydrocarbons (e.g. aminofluorene and acetylaminofluorene) to form mutagens, as compared with control mice injected with saline. A similar extract from mice exposed to 20,000 ppm in air for 8 hr also has enhanced ability to activate aminofluorene as a mutagen. These results imply that the compound may pose a carcinogenic risk by acting as co-carcinogenic enhancer for carcinogen metabolic activation (14).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level $1 \mu\text{g l}^{-1}$ (15).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (16).

Other comments

Reviews on human health effects, experimental toxicology, epidemiology, exposure, workplace experience, environmental effects, ecotoxicology listed (17).

Environmental problems created by chlorofluorocarbons have been reviewed (18).

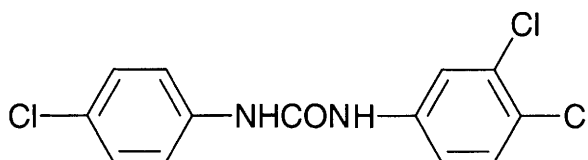
Chlorofluorocarbons are very stable and accumulate in the atmosphere without significant decomposition. They diffuse into the stratosphere where their chlorine atoms react with atmospheric ozone to a significant extent, resulting in a significant depletion of ozone. These compounds are considered to be responsible for the depletion of stratospheric ozone over the South Pole (9).

References

1. McDuffie, B. *Chemosphere* 1981, **10**, 73-82.
2. Howard, P. H. (Ed.) *Handbook of Fate & Exposure Data for Organic Chemicals* 1990, **II**, Lewis Publishers, Chelsea, MI, USA.
3. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, **63**(3), 198-207.
4. *Environmental Properties of Chemicals* 1990, Research Report 91, Ministry of the Environment, Finland.
5. *J. Occup. Med.* 1962, **4**, 262.
6. *Anaesthesia* 1961, **16**, 3.
7. Trochimowicz, H. J. et al *Fundam. Appl. Toxicol.* 1988, **11**(1), 68-75.
8. *Union Carbide Data Sheet* 10th July 1970.
9. *Chemical Safety Data Sheets* 1989, **1**, 322-325, The Royal Society of Chemistry, London, UK.
10. Eriksson, L. et al *Environ. Toxicol. Chem.* 1991, **10**(5), 585-596.
11. Stopps, G. J. *Am. Ind. Hyg. Assoc. J.* 1967, **28**, 43.
12. Taylor, G. J. *J. Am. Med. Assoc.* 1970, **214**, 81.
13. Imbus, H. R. *Arch. Environ. Health* 1972, **24**, 257.

14. Mahurin, R. G. et al *Environ. Res.* 1988, **45**, 101-107.
15. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
16. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; *6th Amendment EEC Directive* 79/831/EEC; *7th Amendment EEC Directive* 91/32/EEC 1991, HMSO, London, UK.
17. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium.
18. Ohkita, T. *Anzen Kogaku* 1988, **27**(6), 328-335 (Japan.) (*Chem. Abstr.* **111**, 63057e)

T270 triclocarban



$C_{13}H_9Cl_3N_2O$

Mol. Wt. 315.59

CAS Registry No. 101-20-2

Synonyms *N*-(4-chlorophenyl)-*N'*-(3,4-dichlorophenyl)urea; 3,4,4'-trichlorocarbanilide; 3,4,4'-trichlorodiphenylurea; TCC; solubacter

EINECS No. 202-924-1

RTECS No. FE 1250000

Uses Bacteriostat in soaps and detergents. Dinsinfectant.

Physical properties

M. Pt. 255-256°C

Ecotoxicity

Invertebrate toxicity

LC₅₀ (48 hr) *Mercenaria mercenaria* 0.032 mg l⁻¹ (1).

Environmental fate

Degradation studies

Biodegradation in sewage and activated sludge: complete biodegradation of 200 µg l⁻¹ within 10 hr (2).

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal mouse 2100 mg kg⁻¹ (3).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (4).

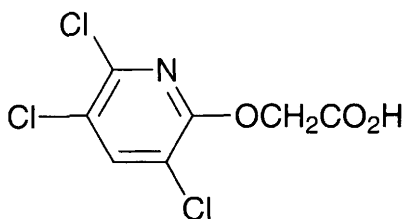
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level 1 µg l⁻¹ (5).

References

1. Davis, H. C. et al *Fish Bull.* 1969, **67**(2), 383-404.
2. Gledhil, W.E. *Water Res.* 1975, **9**, 649-654.
3. *Labo Pharma-Problemes et Techniques* 1979, **27**, 306.
4. Zeiger, E. et al *Environ. Mol. Mutagen.* 1987, **9**(Suppl. 9), 1-109.
5. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T271 triclopyr



C₇H₄Cl₃NO₃

Mol. Wt. 256.47

CAS Registry No. 55335-06-3

Synonyms 3,5,6-trichloro-2-pyridyloxyacetic acid; [(3,5,6-trichloro-2-pyridinyl)oxy]acetic acid

EINECS No. 259-597-3

Uses Herbicide used for control of woody plants and broad-leaved weeds in grassland, uncultivated land, industrial areas, coniferous forests, plantation crops, and rice fields.

Physical properties

M. Pt. 150.5°C **B. Pt.** Decomp. 208°C **Specific gravity** 1.85 at 21°C **Partition coefficient** log P_{ow} 0.42 at pH 5, -0.45 at pH 7, -0.96 at pH 9 **Volatility** v.p. 1.5 × 10⁻⁶ at 25°C

Solubility Water: 0.408 (purified), 7.69 (pH 5), 8.10 (pH 7), 8.22 (pH 9) g⁻¹ at 20°C. Organic solvents: acetone, acetonitrile, dichloromethane, ethyl acetate, hexane, methanol, toluene

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) rainbow trout, bluegill sunfish 117, 148 mg l⁻¹, respectively (1).

Following exposure of bluegill sunfish to 2.5 mg l⁻¹ [¹⁴C]triclopyr, the principal components observed in the tissues were triclopyr, 3,5,6-trichloro-2-pyridinol, 2-methoxy-3,5,6-trichloropyridine and a conjugate. These accounted for 75% of all residues observed (2).

Invertebrate toxicity

EC₅₀ (5 day) *Selenastrum capricornutum* 45 mg l⁻¹ (1).

EC₅₀ (48 hr) *Daphnia magna* 133 mg l⁻¹ (1).

LD₅₀ contact bees > 100 µg bee⁻¹ (1).

Bioaccumulation

Following exposure of crayfish to 1 or 2.5 mg l⁻¹ for 11 days, elimination of accumulated residues was investigated for 36 days. Most of the residue in whole crayfish was present in the shell and haemolymph, primarily as parent triclopyr. The main metabolite in the hepatopancreas was the taurine conjugate of triclopyr. Bioconcentration factors were calculated to be about 1 in whole crayfish and hepatopancreas and about 0.2 in muscle (3).

Environmental fate

Degradation studies

Fairly rapidly degraded in soil by microbial activity, average $t_{1/2}$ 46 days, depending on soil and climatic conditions (1).

Triclopyr degradation rates were determined in laboratory studies on two surface soils and two subsoils from the rice-producing areas of Arkansas. The average $t_{1/2}$ was 138 days (4).

Abiotic removal

Not readily hydrolysed (pH 5-9) (5).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mallard ducks 1698 mg kg⁻¹ (1).

TD₅₀ oral rat 1550 mg kg⁻¹ (6).

LD₅₀ oral rat 630 mg kg⁻¹ (7).

LD₅₀ oral rabbit 550 mg kg⁻¹ (1).

LD₅₀ oral guinea pig 310 mg kg⁻¹ (1).

LD₅₀ dermal rabbits >2000 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

Eight-day dietary LC₅₀ mallard ducks, Japanese quail, bobwhite quail >5000, 3278 and 2935 mg kg⁻¹, respectively (1).

Carcinogenicity and chronic effects

Oral rats, mice (2 yr) no-observed-effect level 3.0, 5.3 mg kg⁻¹, respectively, in diet (1).

Teratogenicity and reproductive effects

Gavage pregnant rats 0, 50, 100 or 200 mg kg⁻¹ day⁻¹ on days 6-15 of gestation. Dose-related signs of maternal toxicity were observed during the treatment period but no teratogenic effects at any dose level. ♂ and ♀ rats fed on diets containing 0, 3, 10 or 30 mg kg⁻¹ day⁻¹ for three generations exhibited no consistent treatment-related effects on reproductive performance, pregnancy, parturition or neonatal survival (8).

Metabolism and toxicokinetics

Oral mice single dose of 3 or 60 mg kg⁻¹ [¹⁴C]triclopyr. Radioactivity was cleared from the plasma of ♂ rats at 3 mg kg⁻¹ in a monoexponential manner, with a first-order elimination half-life of 3.6 hr. Of the administered radioactivity, 89-95% was excreted in the urine, 81-96% of this was unchanged [¹⁴C]triclopyr. Four minor urinary metabolites were also detected. The faeces contained <3% of the administered dose of radioactivity, and expired CO₂ <1% (9).

Single dermal applications of 3.7 mg kg⁻¹ applied to the forearms of five human volunteers were slowly absorbed through the skin, with $t_{1/2}$ 16.8 hr (10).

Following single oral administration of 0.1 or 0.5 mg kg⁻¹ doses to six human volunteers, blood levels peaked at 2-3 hr and declined to undetectable levels by 48 hr. More than 80% of the dose was recovered unchanged in the urine (10).

Irritancy

Mild eye irritant in rabbits (1).

Sensitisation

Non-irritating to skin of rabbits (1).

Other effects

Any other adverse effects

Triclopyr administered to ponies at 60 mg kg⁻¹ produced no clinical signs, but administration at 300 mg kg⁻¹ did produce clinical signs generally characterised by anorexia, central nervous system depression, muscular weakness, gastro-intestinal hypomotility and constipation (proceeding to diarrhoea) (11).

Legislation

WHO Toxicity Class III (12).

EPA Toxicity Class III (1).

ADI 0.005 mg kg⁻¹ body weight (1).

Limited under EC Directive on Drinking Water Quality 80/788/EEC. Pesticides: maximum admissible concentration 0.5 µg l⁻¹ (13).

Included in Schedules 5 and 6 (Release into Water and Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (14).

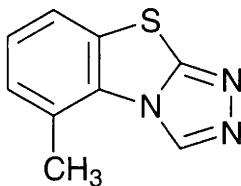
Other comments

In vitro growth tests on five species of ectomycorrhizal fungi (*Hebeloma crustuliniforme*, *Laccaria laccata*, *Thelophora americana*, *T. terrestris*, *Suillus tomentosus*) showed triclopyr to reduce fungal growth significantly, particularly at concentrations > 10 ppm (15).

References

1. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
2. Lickly, T.D. et al *Environ. Int.* 1987, **13**(2), 213-218.
3. Barron, M. G. et al *Drug Metab. Dispos.* 1991, **19**(1), 163-167.
4. Johnson, W. G. et al *Weed Sci.* 1995, **43**(4), 678-684.
5. U.S. Department of Agriculture (U.S. Forest Service). *Pesticide Background Statements. Vol. I: Herbicides* 1984, U.S. Department of Agriculture, Washington, DC, USA.
6. *Fundam. Appl. Toxicol.* 1984, **4**, 872.
7. *Farm Chemicals Handbook* 1983, p.C242, Meister Publishing, 37841 Euclid Av., Willoughby, OH 44094, USA.
8. Hanley, T. R., Jr. et al *Fundam. Appl. Toxicol.* 1984, **4**(5), 872-882.
9. Timchalk, C. et al *Toxicology* 1990, **62**(1), 71-87.
10. Carmichael, N. G. et al *Hum. Toxicol.* 1989, **8**(6), 431-437.
11. Osweiler, G. D. *Proc. Annu. Meet.-Am. Assoc. Vet. Lab. Diagn.* 1983, 26th, 193-201.
12. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
13. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
14. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
15. Chakravarty, P. et al *Eur. J. For. Pathol.* 1987, **17**(4-5), 204-210

T272 tricyclazole



C₉H₇N₃S

Mol. Wt. 189.24

CAS Registry No. 41814-78-2

Synonyms tricyclazone; BEAM; EL-291; 5-methyl-1,2,4-triazolo[3,4b]benzothiazole; 5-methyl-1,2,4-triazolo[3,4b][1,3]benzothiazole

EINECS No. 255-559-5

RTECS No. XZ 5475000

Uses Fungicide.

Physical properties

M. Pt. 187-188°C B. Pt. 275°C Partition coefficient $\log P_{ow}$ 1.40 Volatility v.p. 0.203×10^{-6} mm Hg at 25°C
Solubility Water: 1.6 g l⁻¹. Organic solvents: acetone, methanol, xylene

Occupational exposure

JP-OEL 3 mg m⁻³

Supply classification harmful

Risk phrases Harmful if swallowed (R22)

Safety phrases Keep out of reach of children (if sold to general public) (S2)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bluegill sunfish 16.0, rainbow trout 7.3, goldfish fingerlings 13.5 mg l⁻¹ (1).

Invertebrate toxicity

LC₅₀ *Daphnia* (48 hr) >20 mg l⁻¹; (21 d) 0.96 mg l⁻¹ no observed effect (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 250-315 mg kg⁻¹ (2,3).

LD₅₀ oral mouse 245-250 mg kg⁻¹ (3,4).

LD₅₀ oral mallard duck, bobwhite quail >100 mg kg⁻¹ (3).

LD₅₀ oral dog >50 mg kg⁻¹ (3).

LC₅₀ (1 hr) inhalation rat 0.146 mg l⁻¹ (3).

LD₅₀ percutaneous rat >2000 mg kg⁻¹ (3).

Carcinogenicity and chronic effects

Oral rat (2 yr) 275 mg kg⁻¹ in diet, no observed effect (4).

Oral mouse (2 yr) 400 mg kg⁻¹ in diet, no observed effect (4).

Irritancy

Slight eye irritant; non-irritating to skin (rabbits) (4).

Genotoxicity

Salmonella typhimurium LT-2 TA1535, TA100, TA1538, TA98, TA102 with and without metabolic activation negative (1).

Salmonella typhimurium TA100, TA98, TA1538, TA1537, TA153 and *Escherichia coli* WP2 *hcr* non-mutagenic (5).

Saccharomyces cerevisiae genetic activity test negative (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (6).

Included in Schedule 6 (Release into Land Prescribed Substances) of Statutory Instrument No. 472, 1991 (7).

WHO Toxicity Class II (8).

EPA Toxicity Class II (formulation) (3).

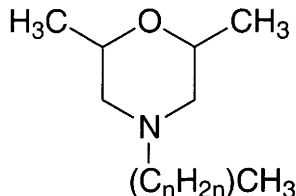
ADI 0.03 mg kg⁻¹ (3).

References

1. Choi, E. J. *Environ. Mutagen. Carcinog.* 1985, 5(1), 11-18.
2. *Agricultural Chemicals Book IV*, 1976, p. 120, Thomson Publications, Fresno, CA, USA.
3. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.

4. *Farm Chemicals Handbook* 1983, Chapter 243, Meister Publishing, 37841 Eclid Ave, Willoughby, OH 44094, USA.
5. Moriya, M. *Mutat. Res.* 1983, **116**, 185-216.
6. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
7. S.I. 1991, No. 472, *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
8. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21

T273 tridemorph



n = 10, 11, 12 (60–70%) or 13

C₁₉H₃₉NO(a_{approx.})

Mol. Wt. 297.52

CAS Registry No. 81412-43-3

Synonyms 2,6-dimethyl-4-tridecyltetrahydro-1,4-oxazine; N-tridecyl-2,6-dimethylmorpholine; 2,6-dimethyl-4-tridecylmorpholine

EINECS No. 246-347-3

RTECS No. QE 2705000

Uses Fungicide.

Physical properties

B. Pt. 134°C at 0.5 mmHg (tech.) **Flash point** 142°C (Pensky-Martens) **Specific gravity** 0.86 (tech.) at 20°C

Partition coefficient log P_{ow} 4.2 at pH 7 and 22°C (1) **Volatility** v.p. 9.0 × 10⁻⁵ mmHg at 20°C

Solubility Water: 1.1 mg l⁻¹ at pH 7 and 20°C. Organic solvents: miscible with acetone, cyclohexane, ethanol, ethyl acetate

Occupational exposure

Supply classification harmful

Risk phrases Harmful in contact with skin and if swallowed (R21/22)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with the eyes – Wear suitable protective clothing and gloves (S2, S25, S36/37)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) trout 3.4 mg l⁻¹ (1).

Invertebrate toxicity

LD₅₀ (24 hr) >2000 µg bee⁻¹ (1).

Mammalian & avian toxicity

Acute data

LD₅₀ quail, duck 1388, >2000 mg kg⁻¹ (1).

LD₅₀ oral rat, rabbit, mouse 650-1560 mg kg⁻¹ (2-4).

LC₅₀ (4 hr) inhalation rat 4500 mg m⁻³ (1).

LD₅₀ dermal rabbit >4000 mg kg⁻¹ (1).

Carcinogenicity and chronic effects

Oral rat, mouse (2 yr) no-adverse-effect level for rats 30 mg kg⁻¹ diet, for mice >90 mg kg⁻¹ diet (1).

Other effects

Any other adverse effects

Inhibits steroid reduction (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (5).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (6).

The log P_{ow} value exceeds the European Community recommended level 3.0 (7).

WHO Toxicity Class II (8).

EPA Toxicity Class III (formulation) (1).

ADI 0.016 mg kg⁻¹ (1).

Other comments

Tridemorph was originally thought to consist only of tridecyl (C₁₃) isomers. The reaction mixture has now been shown to comprise C₁₁ to C₁₄ homologues containing 60-70% of 4-tridecyl isomers, 0.2% C₉ and C₁₅ homologues, and 5% of 2,5-dimethyl isomers (1).

References

1. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
2. *Guide to Chemicals Used in Crop Protection* 1973, 6, 522, Information Canada, Ottawa, Canada.
3. *Vopr. Pitan.* 1981, 39(6), 55.
4. *Pesticide Index* 1976, 5, 229.
5. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
6. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
7. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, Luxembourg.
8. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21

T274 tridymite



O₂Si

Mol. Wt. 60.08

CAS Registry No. 15468-32-3

Synonyms Christensenite; α-tridymite

EINECS No. 239-487-1

RTECS No. VV 7335000

Occurrence Occurs in a number of mineral deposits and can be formed by natural conversion of quartz or amorphous silica. A form of crystalline silica (1).

Occupational exposure

DE-MAK 0.15 mg m⁻³ (respirable fraction of aerosol)
FR-VME 0.05 mg m⁻³ (respirable dust)
SE-LEVL 0.05 mg m⁻³ (respirable dust)
UK-LTEL MEL 0.4 mg m⁻³ (respirable dust)
US-TWA 0.05 mg m⁻³ (respirable fraction)

Mammalian & avian toxicity

Acute data

LD_{Lo} intratracheal rat 200 mg kg⁻¹ (2).

Carcinogenicity and chronic effects

Limited evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2A (3).

Intrathoracic mouse (19 month) single injection of 10 mg in saline. Treated animals developed 1 lung adenocarcinoma and 2 intrapleural lymphoid tumours; 1 lung adenocarcinoma and no lymphoid tumours were seen in controls. Lesions described as lymph node reactive hyperplasia simulating malignancy were found in 19/32 treated mice (1).

Intrapleural rat single injection of 20 mg. 16/32 rats developed malignant lymphomas, histiocytic type, and the mean survival was 525 days. No such tumours were found in 16 ♂ and 16 ♀ controls whose mean survival was 717 days (1).

Genotoxicity

In vitro human lymphocytes plus monocytes sister chromatid exchanges positive, human purified lymphocytes sister chromatid exchanges negative (4).

Other effects

Other adverse effects (human)

Exposure to crystalline silica can cause silicosis, a nodular pulmonary fibrosis caused by the deposition of particles in the lungs (1).

Any other adverse effects

Following intratracheal injection of 50 mg into rats, tridymite was more fibrogenic than cristobalite and quartz. Tridymite-induced nodules reached the maximum grade of fibrosis by 60 days, while those induced by quartz took 240 days (1).

Pure quartz reduced the viability of rat peritoneal macrophages to a greater extent than tridymite. Tridymite is ~8 × more toxic to guinea pig leukocyte cultures than quartz or vitreous silica. Etching of tridymite increased its toxicity to guinea pig peritoneal macrophages (1).

The mortality of rat peritoneal macrophages incubated with tridymite increased from 0 in controls to 79.9% (5).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (6).

Other comments

Reviews on human health effects, experimental toxicology, workplace experience listed (7).

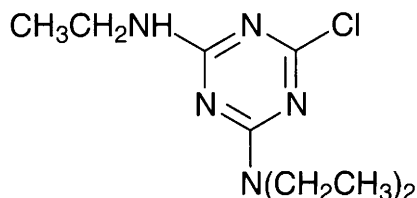
Tridymite, quartz and cristobalite are interrelated and may change their form under different conditions of temperature and pressure; the α, or low-temperature, forms are the most common (1).

References

1. IARC Monograph 1987, 42, 39-143.
2. Br. J. Ind. Med. 1953, 10, 9.

3. IARC Monograph 1987, **Suppl. 7**, 70.
4. Pairon, J. C. et al *Br. J. Ind. Med.* 1990, **47**(2), 110-115.
5. Governa, M. et al *Rapp. ISTISAN* 1988, ISTISAN 88/28, Corso Tero.-Prat. Util. Colt. Cell. Indag. Tossicol., 135-146 (Ital.) (*Chem. Abstr.* **110**, 207307r).
6. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
7. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T275 trietazine



$C_9H_{16}ClN_5$

Mol. Wt. 229.71

CAS Registry No. 1912-26-1

Synonyms 6-chloro-*N,N,N'*-triethyl-1,3,5-triazine-2,4-diamine; *s*-triazine, 2-chloro-4-(diethylamino)-6-(ethylamino)-; Gesafloc

EINECS No. 217-618-3

RTECS No. XY 5425000

Uses Selective herbicide.

Physical properties

M. Pt. 102-103°C

Solubility Water: 20 mg l⁻¹ at 25°C. Organic solvents: acetone, benzene, chloroform, dioxane, ethanol

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) common carp 0.85 mg l⁻¹ (1).

LC₅₀ (24 hr) guppy 5.5 mg l⁻¹ (2).

Invertebrate toxicity

LC₅₀ *Daphnia pulex* >40 mg l⁻¹ (1).

Non-toxic to honey bees (3).

Mammalian & avian toxicity

Acute data

LD₅₀ quail 800 mg kg⁻¹ (2).

LD₅₀ oral rat 2830-4000 mg kg⁻¹ (2).

Sub-acute and sub-chronic data

In 90-day feeding trials, rats receiving 16 mg kg⁻¹ diet showed no ill-effects (2).

Irritancy

Non-irritating to rat skin (2).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (4).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (5).
WHO Toxicity Class Table 5 (6).

References

1. Nishiuchi, Y. et al *Botyu-Kagaku* 1967, 32, 5-11.
2. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
3. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
5. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
6. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21

T276 triethanolamine



C₆H₁₅NO₃

Mol. Wt. 149.19

CAS Registry No. 102-71-6

Synonyms tris(β-hydroxyethyl)amine; 2,2',2''-nitrilotriethanol; nitrilotriethanol; triethylolamine

EINECS No. 203-049-8

RTECS No. KL 9275000

Uses Intermediate in the manufacture of surface active agents, waxes, polishes, herbicides, cement additives. Solvent.

Physical properties

M. Pt. 18-21°C **B. Pt.** 335.4°C **Flash point** 185°C **Specific gravity** 1.1242 at 20°C with respect to water at 4°C **Partition coefficient** log P_{ow} -1.59 (1) **Volatility** v.p. <0.01 mmHg at 20°C; v.den. 5.14

Solubility Water: miscible with water. Organic solvents: acetone, benzene, chloroform, diethyl ether, ethanol, methanol

Occupational exposure

SE-LEVL 5 mg m⁻³

SE-STEL 10 mg m⁻³

US-TWA 5 mg m⁻³

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) goldfish >5000 mg l⁻¹ (2).

5 ppm (24 hr) caused no toxic effects on trout, bluegill sunfish, yellow perch and goldfish (3).

Invertebrate toxicity

LOEC *Scenedesmus quadricauda* 1.8 mg l⁻¹ (4).

LOEC *Microcystis aeruginosa* 47 mg l⁻¹ (5).

Bioaccumulation

A bioconcentration factor of <1 was estimated based on the log P_{ow}. This value and the complete solubility of the compound in water suggest it does not bioconcentrate significantly in aquatic organisms (1).

Environmental fate

Nitrification inhibition

No inhibition of ammonia oxidation by *Nitrosomonas* sp. at 100 mg l⁻¹ (6).

Degradation studies

ThOD 2.04; BOD₅ 0% of ThOD (7).

Abiotic removal

t_{1/2} for triethanolamine vapour reacting with photochemically generated hydroxyl radicals was estimated to be ~4 hr based on an estimated reaction rate constant of 10.4 × 10⁻¹¹ cm³ molecules⁻¹ sec⁻¹ at 25°C and an average ambient hydroxyl concentration of 5 × 10⁵ molecules cm⁻³ (8).

Adsorption capacity on activated carbon 0.067 g g⁻¹ carbon; influent 1000 mg l⁻¹, effluent 670 mg l⁻¹, reduction 33.0% (9).

Adsorption and retention

A soil adsorption coefficient of 3 was estimated based on the log P_{ow}. The value and the complete solubility of the compound in water suggest it would be extremely mobile in soil and would not adsorb significantly to solids and sediments in water (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral guinea pig, mouse 5300, 7400 mg kg⁻¹, respectively (10,11).

LD₅₀ intraperitoneal mouse 1450 mg kg⁻¹ (12).

Sub-acute and sub-chronic data

Oral rat (30 day) 0.005-2.61 g kg⁻¹ in their diet. Responses included reduced growth, altered organ weights, microscopic lesions (tissue unspecified) and death. The NOEL was 0.08 g kg⁻¹ (13).

Dermal guinea pig 8 g kg⁻¹ day⁻¹ 5 days wk⁻¹. The animals died between the second and seventeenth application. Necrosis of the epithelium, and lung and adrenal congestion were observed. The kidneys and liver also showed congestion along with cloudy swelling (14).

Carcinogenicity and chronic effects

The National Toxicology Program tested rats and mice dermally. Equivocal evidence of carcinogenicity in ♂ rats, no evidence of carcinogenicity in ♀ rats, inadequate evidence of carcinogenicity in ♂ mice, some evidence of carcinogenicity in ♀ mice (15).

Oral rat (2 yr) 0%, 1% or 2% in drinking water. Absolute and relative kidney weights increased significantly in a dose-related fashion and kidneys were enlarged, granular on the surface and anaemic in colour. Chronic nephropathy was seen in both ♂ and ♀. Mineralisation of the renal papilla, nodular hyperplasia of the pelvic mucosa, and pyelonephritis with or without papillary necrosis were seen more frequently in treated animals than in controls. A positive trend was seen in the occurrence of hepatic tumours in ♂ and of uterine endometrial sarcomas and renal cell adenomas in ♀. Under the conditions of the study, the authors conclude the compound was not carcinogenic (16).

Oral mice 0%, 0.03% or 0.3% in their diet for life. The total incidence of malignant tumours in treated animals was significantly higher than that observed in controls (target sites unspecified) (17).

Irritancy

Dermal rabbit (24 hr) 560 mg caused mild irritation (18).

10 mg instilled into rabbit eye caused mild irritation (duration unspecified) (19).

Sensitisation

Solutions containing 6% and 15% showed no sensitising properties when applied to the skin of guinea pigs (20).

Genotoxicity

Not mutagenic in any short-term *in vivo* or *in vitro* tests performed by the National Toxicology Program (15).

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (21).

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537, TA1538 with and without metabolic activation negative (22).
Escherichia coli WP2, WP2uvrA with and without metabolic activation negative (22).
Saccharomyces cerevisiae JD1 gene conversion with and without metabolic activation negative (22).
In vitro rat liver cells chromosome assay negative (22).
Drosophila melanogaster sex-linked recessive lethal mutations negative (23).

Other effects

Other adverse effects (human)

Occupational exposure has resulted in allergic contact dermatitis, erythematous vesicular lesions, eczema, contact dermatitis and irritation (24).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (25).

Other comments

Reviews on human health effects, experimental toxicology, epidemiology, ecotoxicology, environmental effects, exposure levels, exposure conditions, workplace experience, safety test data listed (26).

References

- Howard, P. H. (Ed.) *Handbook of Fate & Exposure Data for Organic Chemicals* 1990, II, Lewis Publishers, Chelsea, MI, USA.
- Bridie, A. L. et al *Water Res.* 1979, **13**, 623.
- The Toxicity of 3400 Chemicals to Fish* 1987, EPA560/6-87-002 PB 87-200-275, Washington, DC, USA.
- Bringmann, G. et al *Water Res.* 1980, **14**, 231-241.
- Bringmann, G. et al GWF, *Gas-Wasserfach: Wasser/Abwasser* 1976, **117**(9).
- Hockenbury, M. R. et al *J. Water Pollut. Control Fed.* 1977, **49**(5), 768-777.
- Lund, H. F. *Industrial Pollution Control Handbook* 1971, McGraw-Hill, New York, NY, USA.
- Atkinson, R. *Int. J. Chem. Kinet.* 1987, **19**, 799-828.
- Gusti, D. M. et al *J. Water Pollut. Control Fed.* 1974, **46**(5), 947-965.
- Gig. Zr. Prof. Zabol.* 1982, **26**(8), 53.
- Gig. Sanit* 1964, **29**(11), 25.
- Russ. Chem. Rev.* 1969, **38**, 975.
- Smyth, H. F. et al *Arch. Ind. Hyg. Occup. Med.* 1951, **4**, 122.
- Kindsvatter, V. H. *Ind. Hyg. Toxicol.* 1940, **22**, 206.
- National Toxicology Program Research and Testing Division* 1998, Report No. TR449, NIEHS, Research Triangle Park, NC 27709, USA.
- Maekawa, A. et al *Toxicol. Environ. Health* 1986, **19**, 345.
- Hoshino, H. et al *Cancer Res.* 1978, **38**, 3918.
- Toxicol. Appl. Pharmacol.* 1971, **19**, 276.
- Toxicol. Appl. Pharmacol.* 1980, **55**, 501.
- Kotrodymoua, G. M. *Gig. Sanit.* 1975, **6**, 10.
- Mortelmans, K. et al *Environ. Mutagen.* 1986, **8**(Suppl. 7), 1.
- Dean, B. J. et al *Mutat. Res.* 1985, **153**, 57-77.
- Inoue, K. et al *Mutat. Res.* 1982, **101**, 305.
- Appl. Occup. Environ. Hyg.* 1992, **7**(2), 137-139.
- S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
- ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T277 triethoxysilane



$\text{C}_6\text{H}_{16}\text{O}_3\text{Si}$

Mol. Wt. 164.28

CAS Registry No. 998-30-1

EINECS No. 213-650-7

RTECS No. VV 6682000

Physical properties

B. Pt. 134-135°C Flash point 26°C Specific gravity 0.890

Mammalian & avian toxicity

Acute data

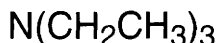
LC₅₀ (2 hr) inhalation mouse 500 mg m⁻³ (1).

LD₅₀ intravenous mouse 180 mg kg⁻¹ (2).

References

1. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
2. U.S. Army Armament Research and Development Command NX 00018, Chemicals Systems Laboratory, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD 21010, USA

T278 triethylamine



$\text{C}_6\text{H}_{15}\text{N}$

Mol. Wt. 101.19

CAS Registry No. 121-44-8

Synonyms *N,N*-diethylethanamine; (diethylamino)ethane; TEA

EINECS No. 204-469-4

RTECS No. YE 0175000

Uses Curing agent for polymers and rubbers. In preparation of quaternary ammonium compounds. Solvent.

Occurrence Occurs naturally in some foods.

Physical properties

M. Pt. -115°C B. Pt. 89-90°C Flash point -6°C (closed cup) Specific gravity 0.723 at 25°C with respect to water at 4°C Partition coefficient log P_{ow} 1.45 Volatility v.p. 50 mmHg at 20°C; v.den. 3.48

Solubility Water: slightly soluble in water >18.7°C, miscible below this temperature. Organic solvents: miscible with diethyl ether, ethanol

Occupational exposure

DE-MAK 1 ppm (4.2 mg m⁻³)

FR-VLE 10 ppm (40 mg m⁻³)

SE-LEVL 2 ppm (8 mg m⁻³)

SE-STEL 10 ppm (40 mg m⁻³)

UK-LTEL 10 ppm (42 mg m⁻³)

UK-STEL 15 ppm (63 mg m⁻³)

US-TWA 1 ppm (4.1 mg m⁻³)

US-STEL 3 ppm (12 mg m⁻³)

UN No. 1296 HAZCHEM Code 3WE Conveyance classification flammable liquid, corrosive

Supply classification highly flammable

Supply classification corrosive

Risk phrases Highly flammable – Harmful by inhalation, in contact with skin and if swallowed – Causes severe burns (R11, R20/21/22, R35)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep in a cool place – Keep away from sources of ignition – No smoking – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Do not empty into drains – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S3, S16, S26, S29, S36/37/39, S45)

Ecotoxicity

Bioaccumulation

A bioconcentration factor of 7.45 was estimated using the log P_{ow} value. This indicates that the compound would not be expected to bioconcentrate in aquatic organisms (1).

Environmental fate

Nitrification inhibition

25-50% inhibition of ammonia oxidation by *Nitrosomonas* sp. at 100 mg l⁻¹; 63% inhibition at 150 mg l⁻¹ (2).

Degradation studies

Degradation by *Aerobacter* 200 mg l⁻¹ at 30°C: parent 100% in 28 hr, mutant 100% in 11 hr (3).
 $t_{1/2}$ in a model river 9.3 hr (1).

Abiotic removal

Reacts rapidly with photochemically produced hydroxyl radicals with $t_{1/2}$ of 4.5 hr (1).

Adsorption and retention

A soil adsorption coefficient of 11-146 was estimated using the log P_{ow} value. This indicates that the compound would not adsorb appreciably to soils and sediments (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird >100 mg kg⁻¹ (4).
LD₅₀ oral rat 460 mg kg⁻¹ (5).
LD₅₀ oral mouse 546 mg kg⁻¹ (6).
LC_{Lo} (4 hr) inhalation rat, guinea pig 1000 ppm (5,7).
LD₅₀ dermal rabbit 570 mg kg⁻¹ (5).

Teratogenicity and reproductive effects

When injected into 3-day chicken embryos caused deaths, malformed embryos and malformations in survivors (8).

Metabolism and toxicokinetics

In humans, following inhalation an average of 24% of the dose was biotransformed into triethylamine *N*-oxide; the parent compound and this metabolite were then quantitatively eliminated in urine (9).
Plasma $t_{1/2}$ was 3 hr for triethylamine and 4 hr for its metabolite triethylamine *N*-oxide (10).

Irritancy

In rats, severe lung irritation, severe eye irritation and corneal injury produced by inhalation of 50 ppm (duration unspecified) (11).
Dermal rabbit (24 hr) 10 mg caused mild irritation and 250 mg instilled into rabbit eye caused mild irritation (duration unspecified) (5).

Sensitisation

Can cause sensitisation in susceptible individuals (11).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (12).

Other effects

Other adverse effects (human)

Visual disturbances attributable to triethylamine exposure have been reported in polyurethane-foam workers, with foggy vision, blue haze, and halo phenomena, but no permanent eye disease (13,14).

Short-term inhalation by humans disrupted central nervous system activity, probably by acting on brain monoamine oxidase activity (11).

Any other adverse effects

Inhalation rat (≤ 28 wk) 25 or 247 ppm caused no cardiotoxicity (15).

156 ppm in air caused the respiratory rate of mice to decrease by 50% (16).

Chronic exposure via inhalation caused lung, kidney and liver damage in rats, together with definite degeneration changes in the heart (11).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (17).

Other comments

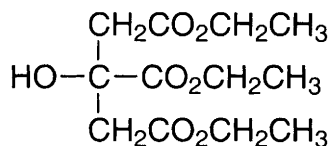
Reviews on human health effects, experimental toxicology, workplace experience, physico-chemical properties, ecotoxicology, epidemiology, environmental effects listed (18).

Autoignition temperature 232°C.

References

1. Howard, P. H. (Ed.) *Handbook of Fate & Exposure Data for Organic Chemicals* 1990, II, Lewis Publishers, Chelsea, MI, USA.
2. Hockenbury, M. R. et al *J. Water Pollut. Control Fed.* 1977, **49**(5), 768-777.
3. Worne, H. E. *Tijdschrift van het BECEWA*, Leige, Belgium.
4. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
5. *AMA Arch. Ind. Health* 1951, **4**, 119.
6. *Hyg. Sanit.* 1965, **30**, 351.
7. *J. Ind. Hyg. Toxicol.* 1948, **30**, 2.
8. Korhonen, A. et al *JAT, J. Appl. Toxicol.* 1983, **3**(2), 112-117.
9. Aakesson, B. et al *Br. J. Ind. Med.* 1988, **45**(4), 262-268.
10. Aakesson, B. et al *Toxicol. Appl. Pharmacol.* 1989, **100**(3), 529-538.
11. *Chemical Safety Data Sheets* 1988, **1**, 326-328, The Royal Society of Chemistry, London, UK.
12. Zeiger, E. et al *Environ. Mutagen.* 1987, **11**(Suppl. 9), 1-109.
13. Aakesson, B. *Int. Arch. Occup. Environ. Health* 1986, **57**(4), 297-302.
14. Aakesson, B. *Br. J. Ind. Med.* 1985, **42**(12), 848-850.
15. Lynch, D. W. et al *Toxicol. Ind. Health* 1990, **6**(3-4), 403-414.
16. Gagnaire, F. et al *J. Appl. Toxicol.* 1989, **9**(5), 301-304.
17. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
18. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T279 triethyl citrate



$\text{C}_{12}\text{H}_{20}\text{O}_7$

Mol. Wt. 276.29

CAS Registry No. 77-93-0

Synonyms ethyl citrate; citric acid, triethyl ester; 1,2,3-propanetricarboxylic acid, 2-hydroxy-, triethyl ester; Citroflex 2; Citrofol A1; TEC; Uniplex 80

EINECS No. 201-070-7

RTECS No. GE 8050000

Uses Plasticiser for polyvinyl chloride.

Physical properties

M. Pt. -55°C **B. Pt.** 127°C at 1 mmHg **Flash point** 155°C **Specific gravity** 1.136 at 25°C

Volatility v.p. 1 mmHg at 107°C

Solubility Organic solvents: miscible with diethyl ether, ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 5900 mg kg⁻¹ (1).

LD₅₀ oral cat 35,000 mg kg⁻¹ (2).

LC₅₀ (6 hr) inhalation rat 1300 ppm (2).

LD₅₀ intraperitoneal rat 4 g kg⁻¹ (1).

LD₅₀ intraperitoneal mouse 1750 mg kg⁻¹ (3).

LD₅₀ subcutaneous rat 6600 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

Rats tolerated inhalation of 296 ppm 6 hr day⁻¹ for 62 days without notable effects. Cats tolerated oral doses of 0.25 ml kg⁻¹ day⁻¹ for 8 wk; mild symptoms after the fourth or fifth dose consisted of weakness, ataxia and depression (4).

Intraperitoneal mice (14 day) 350 mg kg⁻¹ day⁻¹ produced no significant effect on weight gain or haematology (4).

Other comments

Reviews on human health effects, experimental toxicology listed (5).

References

1. *Iyakuhin Kenkyu* 1985, **16**, 214.
2. *Food Cosmet. Toxicol.* 1979, **17**, 357.
3. *J. Pharm. Sci.* 1964, **53**, 774.
4. Clayton, G. D. et al (Eds.) *Patty's Industrial Hygiene and Toxicology* 3rd ed., 191, **2A**, John Wiley & Sons, New York, NY, USA.
5. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T280 triethylene glycol



$\text{C}_6\text{H}_{14}\text{O}_4$

Mol. Wt. 150.17

CAS Registry No. 112-27-6

Synonyms 2,2'-ethylenedioxydiethanol; glycol bis(hydroxyethyl) ester; ethanol, 2,2'-[1,2-ethanediy]bis(oxy)]bis-; Trigen; Trigol

EINECS No. 203-953-2

RTECS No. YE 4550000

Uses Drying agent. Organic synthesis. Oil additive. Plasticiser. Solvent.

Physical properties

M. Pt. -7.3°C B. Pt. 285°C Flash point 227°C Specific gravity 1.122 at 25°C with respect to water at 25°C

Partition coefficient $\log P_{\text{ow}} -2.08$ (calc.) (1) Volatility v.p. 1 mmHg at 114°C ; v.den. 5.17

Solubility Water: miscible. Organic solvents: benzene, diethyl ether, ethanol

Ecotoxicity

Fish toxicity

LC₅₀ (7 day) guppy 62,600 mg l⁻¹ (2).

LC₅₀ (96 hr) bluegill sunfish, inland silverside >10,000 mg l⁻¹ (3).

LC₅₀ (96 hr) fathead minnow 59,900-77,400 mg l⁻¹ (4).

Invertebrate toxicity

EC₅₀ (5 min) *Photobacterium phosphoreum* 32,850 ppm Microtox test (5).

Toxicity threshold, cell multiplication inhibition test, *Pseudomonas putida* 320 mg l⁻¹, *Scenedesmus quadricauda* >10,000 mg l⁻¹, *Entosiphon sulcatum* >10,000 mg l⁻¹ (6).

Environmental fate

Degradation studies

COD 1.57 mg O₂ l⁻¹; BOD₅ 0.03 mg O₂ l⁻¹ (1.4% of ThOD); BOD₁₀ 0.50 mg O₂ l⁻¹ (7,8).

Abiotic removal

Reaction with photochemically produced hydroxyl radicals in the atmosphere, estimated t_{1/2} 11.5 hr (9).

Adsorption by activated carbon 0.105 g g⁻¹ carbon (10).

Adsorption and retention

Estimated K_{oc} of 2 indicates that adsorption to soil and sediments is unlikely (11).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, rabbit, guinea pig 7900-22,000 mg kg⁻¹ (12,13).

LD₅₀ intravenous rat, guinea pig, rabbit 1.9-11.7 mg kg⁻¹ (13).

LD₅₀ intraperitoneal mouse 8140 mg kg⁻¹ (14).

Sub-acute and sub-chronic data

Oral rat (30 day) 5000-8000 mg kg⁻¹ caused no adverse effects (15).

Carcinogenicity and chronic effects

Oral rat (2 yr) 3000-4000 mg kg⁻¹ day⁻¹ caused no adverse effects (15).

Teratogenicity and reproductive effects

Oral rat 4500 mg kg⁻¹ caused no teratogenic effects (exposure unspecified) (13).

Subcutaneous rat, mouse, rabbit 2250 mg kg⁻¹ caused no teratogenic effects (exposure unspecified) (13).

Oral mouse lowest toxic dose, reproductive effects, 90,000 mg kg⁻¹ day⁻¹ on days 7-14 of gestation (16).

Metabolism and toxicokinetics

In rats and rabbits, excreted principally in the urine unchanged and possibly as the mono- and dicarboxylic acid derivatives of triethylene glycol. Little if any was eliminated in the conjugated form. 2-5% was eliminated in faeces and 1% in expired air (17).

Irritancy

Dermal rabbit (24 hr) 500 mg caused moderate irritation (18).

Genotoxicity

In vivo rat bone marrow chromosomal aberrations positive (19).

Other effects

Any other adverse effects

Intraperitoneal rat, changes in alanine aminotransferase activity in the blood serum and liver correlated with the extent of liver damage and/or stimulation of the enzyme formation in hepatocytes (dosage not specified) (20).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (21).

Other comments

Environmental fate reviewed (22).

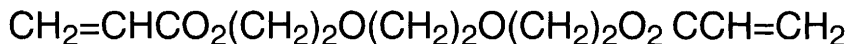
Reviews on human health effects, experimental toxicology, physico-chemical properties listed (23).

Autoignition temp 360°C.

References

1. Verschuieren, K. *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, 1152-1153, Van Nostrand Reinhold, New York, NY, USA.
2. Konemann, W. H. *Quantitative Structure-Activity Relationships for Kinetics and Toxicity of Aquatic Pollutants and their Mixtures in Fish* 1979, Univ. Utrecht, Netherlands.
3. Dawson, G. W. et al *J. Haz. Mat.* 1975, **1** 303-318.
4. Geiger, D. L. et al (Eds.) *Acute Toxicities of Organic Chemicals to Fathead Minnows* 1988, IV, University of Wisconsin – Superior, USA.
5. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
6. Bringmann, G. et al *Water Res.* 1980, **14**, 231-241.
7. *Shell Industrie Chemicalien Gids* 1 January 1975, Shell Nederland Chemie, 's-Gravenhague, Netherlands.
8. Swope, H. G. et al *Sewage Ind. Wastes Eng.* 1950, **21**, 467.
9. Atkinson, R. *Inter. J. Chem. Kinet.* 1987, **19**, 799-828.
10. Guisti, D. M. et al *J. Water Pollut. Control Fed.* 1974, **46**(5), 947-965.
11. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
12. *J. Ind. Hyg. Toxicol.* 1946, **28**, 40.
13. Sterger, et al *Arzneim.-Forsch.* 1968, **18**, 1536.
14. *Fed. Am. Soc. Exp. Biol. Proc.* 1947, **6**, 342.
15. Fitzhugh, O. G. et al *J. Ind. Hyg. Toxicol.* 1948, **28**, 40.
16. *Environ. Health Perspect.* 1984, **57**, 141.
17. McKennis, H. et al *Toxicol. Appl. Pharmacol.* 1962, **4**, 411.
18. *Food Cosmet. Toxicol.* 1979, **17**, 913.
19. Barilyak, I. R. et al *Fiziol. Akt. Veshchestva* 1987, **19**, 3-5 (Russ.) (*Chem. Abstr.* **108**, 2018j).
20. Korkah, V. I. *Gig. Sanit.* 1981, (11), 86-87 (Russ.) (*Chem. Abstr.* **108**, 50727m).
21. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
22. Howard, C. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1993, **4**, 546-551.
23. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T281 triethylene glycol diacrylate



$\text{C}_{12}\text{H}_{18}\text{O}_6$

Mol. Wt. 258.27

CAS Registry No. 1680-21-3

Synonyms 1,2-ethanediylbis(oxy-2,1-ethanediyl 2-propenoate); 2,2'-(ethylenedioxy)diethyl diacrylate

EINECS No. 216-853-9

RTECS No. AS 8150000

Uses Manufacture of polymers.

Physical properties

B. Pt. 140-150°C at 60 mmHg Specific gravity 1.113 at 20°C

Occupational exposure

Supply classification irritant

Risk phrases Irritating to eyes and skin – May cause sensitisation by skin contact (R36/38, R43)

Safety phrases Keep out of reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – After contact with skin, wash immediately with plenty of water (S2, S26, S28)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 500, 700 mg kg⁻¹, respectively (1).

LD₅₀ dermal rabbit 1900 mg kg⁻¹ (2).

Carcinogenicity and chronic effects

Dermal mouse (80 wk) 1000 mg kg⁻¹ 2 × wk⁻¹ caused skin ulceration. 5/50 treated mice developed benign or malignant skin tumours. 20/50 died during the study. Decrease in testicular weight was also reported (3).

Irritancy

Dermal rabbit (24 hr) 500 mg caused severe irritation and 100 mg (exposure rate unspecified) instilled into rabbit eye caused severe irritation (2).

Sensitisation

Sensitisation has been reported in case control studies, although no potential was identified in skin sensitisation tests (3).

Genotoxicity

Salmonella typhimurium Ames test, with and without metabolic activation negative (strains not specified) (3).

In vitro mouse lymphoma mutagenicity assay with and without metabolic activation positive (endpoint not specified) (3).

Other comments

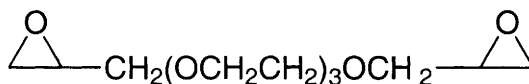
Toxicity of multifunctional acrylates based on eye and skin irritation testing reviewed (3).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (4).

References

1. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals Under Single Exposure* 1982, 115, CIP, Moscow, USSR.
2. *Report* 1981, US EPA 8 EHQ-0981-0410, Office of Pesticides and Toxic Chemicals, Washington DC, USA.
3. Andrews, L. S. et al *J. Toxicol. Environ. Health* 1986, 19(2), 149-164.
4. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T282 triethylene glycol diglycidyl ether



C₁₂H₂₂O₆

Mol. Wt. 262.30

CAS Registry No. 1954-28-5

Synonyms 2,2'-(2,5,8,11-tetraoxa-1,12-dodecanediyl)bisoxyrane; 1,2-bis[2-(2,3-epoxypropoxy)ethoxy]ethane; 1,2:15,16-diepoxy-4,7,10,13-tetraoxahexadecane; Etoglucide

EINECS No. 217-784-7

RTECS No. XF 0700000

Uses Antineoplastic agent.

Physical properties

M. Pt. -15°C to -11°C B. Pt. 133-149°C at 0.1 mmHg Specific gravity 1.1312 at 20°C

Mammalian & avian toxicity

Acute data

LD₅₀ intravenous rat ~700 mg kg⁻¹ (1).

Intravenous doses of 700 mg kg⁻¹ caused death in rats within 2-3 days; following doses of 1200 mg kg⁻¹ death occurred within hours (1).

Intravenous doses of 800 and 500 mg kg⁻¹ to rats and dogs, respectively, resulted in necrosis of the renal tubular epithelium and of the adrenal cortex and intestinal epithelium (1).

Intradermal injections caused severe necrosis in guinea pigs (doses unspecified) (1).

Sub-acute and sub-chronic data

Intravenous dog 100-200 mg kg⁻¹ caused virtual disappearance of neutrophils from the blood after 9 days.

Lymphocyte counts fell by 50%, but erythrocytes and platelets remained constant. The appearance of polychromatic and nucleated red cells on day 14 showed that erythropoiesis was affected (1).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, limited evidence of carcinogenicity to animals, IARC classification group 3 (2).

Intraperitoneal mice (39 wk) 3 × wk⁻¹ for 4 wk total dose 7.2, 3.6, 0.9, 0.22 or 0.06 g kg⁻¹ body weight. Pulmonary tumours were seen in 12/17, 9/24, 14/29, 14/28 and 4/29 mice, respectively (3).

Teratogenicity and reproductive effects

Testicular atrophy and decreased spermatogenic activity were seen in mice in a 39 wk study following intraperitoneal injections (dose unspecified) (3).

Metabolism and toxicokinetics

Following intravenous or subcutaneous administration to rats, 75% of the dose was excreted in the urine as triethyleneglycol-bis-2,3-dihydroxypropyl ether together with a trace of the corresponding mono-diol and two sulfur-containing metabolites, provisionally identified as a hydroxymercapturic acid and an olefinic mercapturate derived from the hydroxy mercapturate by dehydration. A triethylene glycol diglycidyl ether glutathione conjugate and the corresponding cysteinylglycine and cysteine conjugates were excreted into the bile (4).

Irritancy

Dermal rabbit (24 hr) 10 mg caused mild irritation (5).

Genotoxicity

Salmonella typhimurium TA98, TA100 with and without metabolic activation positive (6).

Other effects

Other adverse effects (human)

Side-effects leucopenia and temporary dysuria (1).

Haematological depression has been produced in cancer patients injected with 150-250 mg kg⁻¹ body weight (1).

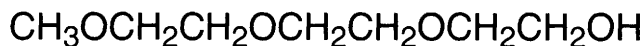
Other comments

Reviews on human health effects, experimental toxicology, exposure listed (7).

References

1. IARC Monograph 1976, 11 209-214.
2. IARC Monograph 1987, **Suppl. 7**, 73.
3. Shimkin, M. B. J. *Natl. Cancer Inst.* 1966, **36**, 915-935.
4. James, S. P. et al *Xenobiotica* 1971, **1**, 43-53.
5. *Am. Ind. Hyg. Assoc. J.* 1962, **23**, 95.
6. Glatt, H. et al *Mutat. Res.* 1983, **11(2)**, 99-118.
7. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T283 triethylene glycol monomethyl ether



C₇H₁₆O₄

Mol. Wt. 164.20

CAS Registry No. 112-35-6

Synonyms 2-[2-(2-methoxyethoxy)ethoxy]ethanol; Dowanol TMAT; methoxytriethylene glycol; methoxitriglycol; triglycol monomethyl ether; 3,6,9-trioxadecanol

EINECS No. 203-962-1

RTECS No. KL 6390000

Uses Solvent.

Physical properties

M. Pt. -44°C **B. Pt.** 122°C at 10 mmHg **Flash point** 118°C (open cup) **Specific gravity** 1.026 at 20°C

Solubility Water: miscible

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 11,300 mg kg⁻¹ (1).

LD₅₀ dermal rabbit 7100 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

Dermal rabbit, (21 days) 1000 mg kg⁻¹ day⁻¹ did not produce systemic toxicity. The low rate of dermal adsorption may have played a role in this outcome (2).

Teratogenicity and reproductive effects

Oral rat, 100 mg kg⁻¹ day⁻¹ on days 6-15 of gestation did not cause maternal or foetal toxicity or any teratogenic effects (2).

Irritancy

Dermal rabbit (24 hr) 10 mg caused mild irritation (1).

500 mg instilled into rabbit eye for 24 hr caused mild irritation (3).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (4).

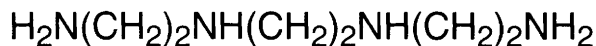
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (5).

References

1. *Am. Ind. Hyg. Assoc. J.* 1962, 23, 95.
2. Leber, A. P. et al *J. Am. Coll. Toxicol.* 1990, 9(5), 507-515.
3. Marhold, J. V. *Prehled Prumyslove Toxikologie: Organické Latky* 1986, Prague, Czechoslovakia.
4. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
5. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T284 triethylenetetramine



$\text{C}_6\text{H}_{18}\text{N}_4$

Mol. Wt. 146.24

CAS Registry No. 112-24-3

Synonyms 3,6-diazaoctane-1,8-diamine; *N,N'*-bis(2-aminoethyl)-1,2-ethanediamine; 1,4,7,10-tetraazadecane; Araldite hardener HY951; trien; trientine; TETA; Texlin 300

EINECS No. 203-950-6

RTECS No. YE 6650000

Uses Catalyst. Chelating agent. Corrosion inhibitor. Cross-linking agent for epoxy resins. Vulcanising agent. Treatment of Wilson's disease.

Physical properties

M. Pt. 12°C **B. Pt.** 266-267°C **Flash point** 143°C **Specific gravity** 0.982 at 20°C

Volatility v.p. <0.01 mmHg at 20°C; v.den. 5.1

Solubility Water: miscible. Organic solvents: acetone, benzene, diethyl ether, ethanol

Occupational exposure

SE-LEVL 1 ppm (6 mg m⁻³)

SE-STEL 2 ppm (12 mg m⁻³)

UN No. 2259 **HAZCHEM Code** 2X **Conveyance classification** corrosive substance

Supply classification corrosive

Risk phrases Harmful in contact with skin – Causes burns – May cause sensitisation by skin contact – Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R21, R34, R43, R52/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S26, S36/37/39, S45)

Ecotoxicity

Bioaccumulation

Confirmed to be non- or low-accumulative (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird >101 mg kg⁻¹ (2).

LD₅₀ oral rat 2.5 g kg⁻¹ (3).

LD₅₀ oral mouse 1.6 g kg⁻¹ (4).

LD₅₀ oral rabbit 5.5 g kg⁻¹ (4).

LD₅₀ dermal rabbit 805 mg kg⁻¹ (5).

LD₅₀ intravenous mouse 350 mg kg⁻¹ (6).

Carcinogenicity and chronic effects

Dermal mouse, 0 or 25% applied 3 × wk⁻¹ until death. 20/50 mice had hyperkeratosis and 13 had necrosis of the epidermis, both indicative of skin irritation. The mortality rate was not significantly different from controls. No treatment-related skin tumours were observed and there was no increase in the incidences of internal tumours. The authors concluded that the compound was not oncogenic under the conditions of these studies (7).

Teratogenicity and reproductive effects

Rats were fed with a diet containing 0.17, 0.83 or 1.66% triethylenetetramine during pregnancy. The frequency of resorptions and abnormal foetuses at term increased with increasing levels of the compound. Maternal and foetal tissue copper levels decreased in a dose-related manner, while maternal kidney and foetal liver zinc levels increased (8).

Metabolism and toxicokinetics

Oral rat, 42% and 22.5% absorbed in the jejunum and ileum, respectively, within 1 hr. Absorption appeared to be by permeation across the plasma membrane of the intestinal epithelial cells. The compound became bound to the brush border membrane of the rat ileum in the absence of inorganic ions such as Na⁺, K⁺, Ca²⁺, Mg²⁺ and Cu²⁺. The urinary excretion of unchanged substance during 24 hr was 3.5% of the orally administered dose. Total urinary excretion, including metabolites, was 35.7% in 24 hr (9).

Irritancy

Dermal rabbit 490 mg caused severe irritation, and 29 mg instilled into rabbit eye caused severe irritation (exposure unspecified) (10).

Owing to its strong alkalinity, the compound (in liquid and vapour forms) is irritating to skin and mucous membranes (11).

Sensitisation

A sensitizer, capable of causing allergic dermatitis (11).

Workers in an electrical equipment factory suffered marked sensitisation, which showed itself as serious skin lesions. Vesicular papular eczema, localised particularly on the hands, forearms and genital and inguinal regions, together with facial oedema, were seen (12).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with and without metabolic activation positive (13).

Other effects

Other adverse effects (human)

Symptoms of inhalation exposure include a burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. Inhalation may be fatal due to bronchial spasm, inflammation and oedema. Chronic exposure, through inhalation or skin absorption may cause anaemia, anorexia, weight loss and cutaneous lesions. Exposure to hot vapour causes itching of the face with erythema and oedema (11).

Any other adverse effects

Hepatotoxicity is due to chelating properties, demonstrated by inhibition of copper superoxide dismutase activity in rat liver (14).

Rats survived exposure to saturated vapour for a maximum of 4 hr (15).

Other comments

Reviews on human health effects, experimental toxicology, workplace experience, environmental effects, ecotoxicology, exposure levels, physico-chemical properties listed (16).

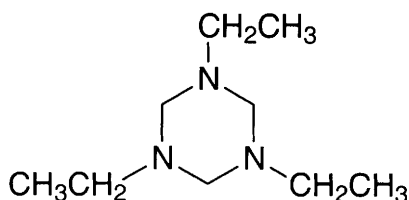
Can form explosive mixtures with nitric acid (11).

Autoignition temperature 337.8°C.

References

1. *The list of the existing chemical substances tested on biodegradability by microorganisms or bioaccumulation in fish body* 1987, Chemicals Inspection & Testing Institute, Japan.
2. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-383.
3. Spitz, R. D. *Kirk-Othmer Encyclopedia of Chemical Technology* 3rd ed., 1979, 7, 580-609, Wiley Interscience, New York, NY, USA.
4. *Khig. Zdraveopaz.* 1979, **22**, 179.
5. *J. Ind. Hyg. Toxicol.* 1949, **31**, 60.
6. *Eur. J. Med. Chem.* 1984, **19**, 425.
7. DePass, L. R. et al *Fundam. Appl. Toxicol.* 1987, **9**(4), 807-811.
8. *Proc. Soc. Exp. Biol. Med.* 1983, **173**(4), 598-605.
9. Kobayashi, M. et al *Yakugaku Zasshi* 1990, **110**(10), 759-63 (Japan.) (*Chem. Abstr.* **114**, 17070t).
10. *Union Carbide Data Sheet* 12 December 1966, New York, NY, USA.
11. *Chemical Safety Data Sheets* 1990, 3, 273-276, The Royal Society of Chemistry, London, UK.
12. Pletscher, A. et al *Z. Unfallmed. Berufskr.* 1954, **47**, 163.
13. Mortelmans, K. et al *Environ. Mutagen.* 1986, **8**(Suppl. 7), 1-119.
14. Ishiyama, H. et al *Pharmacol. Toxicol. (Copenhagen)* 1991, **69**(3), 215-217.
15. Smyth, J. C. et al *J. Ind. Hyg. Toxicol.* 1949, **31**, 60-62.
16. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T285 1,3,5-triethylhexahydro-s-triazine



C₉H₂₁N₃

Mol. Wt. 171.29

CAS Registry No. 7779-27-3

Synonyms 1,3,5-triethylhexahydro-1,3,5-triazine; triethyltrimethylenetriamine; Vancide

EINECS No. 231-924-4

RTECS No. XY 9275000

Physical properties

B. Pt. 207-209°C Flash point 70°C Specific gravity 0.89 at 25°C

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 316 mg kg⁻¹ (1).

LD₅₀ oral mouse 370 mg kg⁻¹ (2).

LD_{Lo} dermal rabbit 2000 mg kg⁻¹ (2).

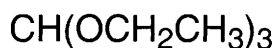
Irritancy

100 mg instilled into rabbit eye for 2 sec caused severe irritation (3).

References

1. *Ind. Med. Surgery* 1970, **39**, 56.
2. *Toxicol. Appl. Pharmacol.* 1967, **10**, 404.
3. *Drug Chem. Toxicol.* 1978, **1**(1), 1

T286 triethyl orthoformate



$\text{C}_7\text{H}_{16}\text{O}_3$

Mol. Wt. 148.20

CAS Registry No. 122-51-0

Synonyms ethyl orthoformate; triethoxymethane; 1,1',1'-(methylidyne)tris(oxy)tris(ethane); orthoformic acid, ethyl ester; Aethon; Ethone

EINECS No. 204-550-4

RTECS No. RM 6475000

Uses Acetylating agent. Catalyst. Drying agent. Cough suppressant.

Physical properties

M. Pt. -76°C B. Pt. 146°C Flash point 30°C (closed cup) Specific gravity 0.895 at 20°C with respect to water at 20°C Volatility v.p. 10 mmHg at 40.5°C ; v.den. 5.11

Occupational exposure

UN No. 2524 HAZCHEM Code 2 $\frac{+}{-}$ Conveyance classification flammable liquid

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 2920 mg kg⁻¹ (1).
LC_{Lo} (8 hr) inhalation rat 4000 ppm (2).
LD₅₀ dermal rabbit 20,000 mg kg⁻¹ (2).
LD₅₀ subcutaneous rabbit 20,000 mg kg⁻¹ (3).

Irritancy

Dermal rabbit (24 hr) 500 mg caused mild irritation and 100 mg instilled into rabbit eye (24 hr) caused moderate irritation (1).

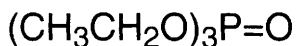
Other comments

Physical properties, safety precautions and toxicity reviewed (4).

References

1. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, **44**, Prague, Czechoslovakia.
2. *AMA Arch. Ind. Hyg. Occup. Med.* 1951, **4**, 119.
3. *Food Cosmet. Toxicol.* 1979, **17**, 917.
4. *Chemical Safety Data Sheets* 1992, **5**, 130-132, The Royal Society of Chemistry, London, UK

T287 triethyl phosphate



$\text{C}_6\text{H}_{15}\text{O}_4\text{P}$

Mol. Wt. 182.16

CAS Registry No. 78-40-0

Synonyms ethyl phosphate; phosphoric acid, triethyl ester

EINECS No. 201-114-5

RTECS No. TC 7900000

Uses Ethylating agent. Used to prepare insecticides.

Physical properties

M. Pt. -56.5°C B. Pt. $215\text{--}216^\circ\text{C}$ Flash point 115°C Specific gravity 1.0725 at 19°C Volatility v.p. 1 mmHg at 39.6°C ; v.den. 6.28

Solubility Organic solvents: diethyl ether, ethanol

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed (R22)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with the eyes (S2, S25)

Ecotoxicity

Bioaccumulation

Confirmed to be non- or low-accumulative (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 1500 mg kg⁻¹ (2).

LD_{Lo} oral guinea pig, rat 1600 mg kg⁻¹ (3).

LD_{Lo} intraperitoneal guinea pig, rat 800 mg kg⁻¹ (3).

LD₅₀ intraperitoneal mouse 485 mg kg⁻¹ (4).

LD_{Lo} intravenous rat 1000 mg kg⁻¹ (5).

Inhalation rat 2000 ppm for 6 hr caused 3/3 deaths, weakness and gasping respiration (6).

Sub-acute and sub-chronic data

Intraperitoneal rat (37 day) 400 mg kg⁻¹ day⁻¹ caused peritoneal irritation, ascites and anaesthesia, but no paralysis (6).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (7).

Drosophila melanogaster wing spot test positive for small single spots, ambiguous for large single and twin spots (8).

Other effects

Any other adverse effects

Sedative in rats (6).

Legislation

The recommended maximum permissible concentration in Russian reservoirs is 0.3 mg l⁻¹ (9).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties, ecotoxicology, environmental effects, exposure levels listed (10).

References

1. *The list of the existing chemical substances tested on biodegradability by microorganisms or bioaccumulation in fish body* 1987, Chemicals Inspection & Testing Institute, Japan.
2. Marhold, J. V. *Prehled Prumyslove Toxikologie: Organicke Latky* 1986, Prague, Czechoslovakia.
3. Deichmann, W. B. *Toxicology of Drugs and Chemicals* 1969, Academic Press, New York, NY, USA.
4. *Therapie* 1960, **15**, 237.
5. *Nature* 1975, **179**, 154.
6. Clayton, G. D. et al (Eds.) *Patty's Industrial Hygiene and Toxicology* 3rd ed., 1981, **2A**, John Wiley & Sons, New York, NY, USA.
7. Zeiger, E. et al *Environ. Mutagen.* 1987, **9**(Suppl. 9), 1-109.
8. Graf, U. et al *Mutat. Res.* 1989, **222**, 359-373.
9. Sakhnovskaya, N. N. et al *Gig. Sanit.* 1991, (5), 17-19 (Russ.) (*Chem. Abstr.* **115**, 108032u).
10. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T288 triethyl phosphite



$\text{C}_6\text{H}_{15}\text{O}_3\text{P}$

Mol. Wt. 166.16

CAS Registry No. 122-52-1

Synonyms phosphorous acid, triethyl ester; triethoxyphosphine; TEP-HP

EINECS No. 204-552-5

RTECS No. TH 1130000

Physical properties

B. Pt. 156°C Flash point 54°C Specific gravity 0.969

Occupational exposure

UN No. 2323 HAZCHEM Code 3Y Conveyance classification flammable liquid

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 3200 mg kg⁻¹ (1).

Irritancy

Dermal mammal 500 mg caused mild irritation and 100 mg instilled into the eye also caused mild irritation (species and duration unspecified) (2).

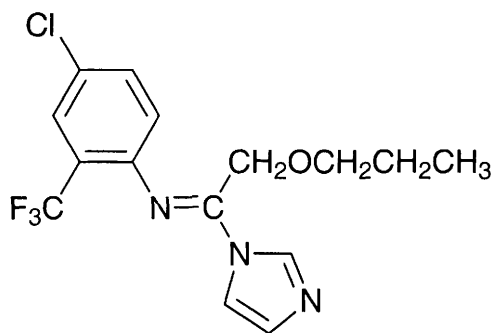
Other comments

Reviews on human health effects, experimental toxicology, environmental effects, ecotoxicology, exposure levels, workplace experience listed (3).

References

1. Lewis, R. J. (Ed.) *Sax's Dangerous Properties of Industrial Materials* 8th ed., 1992, Van Nostrand Reinhold, New York, NY, USA.
2. *Medycyna Pracy* 1978, **29**, 393.
3. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T289 triflumizole



C₁₅H₁₅ClF₃N₃O

Mol. Wt. 345.75

CAS Registry No. 99387-89-0

Synonyms (E)-4-chloro- α,α,α -trifluoro-N-(1-imidazol-1-yl-2-propoxyethylidene)-o-toluidine;
(E-1-[1[[4-chloro-2-(trifluoromethyl)phenyl]imino]-2-propoxyethyl]-1H-imidazole
Uses Fungicide.

Physical properties

M. Pt. 63.5°C **Partition coefficient** log P_{ow} 1.4 at 25°C **Volatility** v.p. 0.186 mPa at 25°C
Solubility Water: 12.5 g/l at 20°C. Organic solvents: acetone, chloroform, hexane, methanol, xylene

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) carp 1.26 mg l⁻¹ (1).

Invertebrate toxicity

EC₅₀ (3 hr) *Daphnia magna* 9.7 mg l⁻¹ (1).

LD₅₀ honey bees 0.14 mg bee⁻¹ (1).

Environmental fate

Degradation studies

In clay soil DT₅₀ 14 days (1).

Abiotic removal

The metabolite (E-4-chloro- α,α,α -trifluoro-N-(1-amino-1-yl-2-propoxyethylidene)-o-toluidine is formed by photolytic degradation (2).

Adsorption and retention

K_{oc} 1083-1663 (1).

Mammalian & avian toxicity

Acute data

LD₅₀ ♂ Japanese quail 2467, ♀ Japanese quail 4308 mg kg⁻¹ (1).

LD₅₀ oral ♂ rats 715, ♀ rats 695 mg kg⁻¹ (1).

LC₅₀ (4 hr) inhalation rats >3.2 mg l⁻¹ air (1).

LD₅₀ dermal rats >5000 mg kg⁻¹ (1).

Carcinogenicity and chronic effects

Oral rats (2 yr) no-observed-effect level 3.7 mg kg⁻¹ diet (1).

Legislation

WHO Toxicity Class III (2).

EPA Toxicity Class III (1).

Limited under EC Directive on Drinking Water Quality 80/788/EEC. Pesticides: maximum admissible concentration 0.5 µg l⁻¹ (3).

Included in Schedules 5 and 6 (Release into Water and Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (4).

References

1. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
2. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
4. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T290 trifluoroacetic acid



C₂HF₃O₂

Mol. Wt. 114.02

CAS Registry No. 76-05-1

Synonyms perfluoroacetic acid; trifluoroethanoic acid

EINECS No. 200-929-3

RTECS No. AJ 9625000

Uses In organic synthesis. Solvent.

Physical properties

M. Pt. -15.4°C B. Pt. 72.4°C Specific gravity 1.5351 at 20°C Volatility v.p. 191 mm Hg at 37°C

Solubility Organic solvents: miscible with acetone, benzene, diethyl ether, hexane, ethanol

Occupational exposure

UN No. 2699 HAZCHEM Code 2X Conveyance classification corrosive substance

Supply classification corrosive

Risk phrases Harmful by inhalation – Causes severe burns (R20, R35)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep container in a well ventilated place – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Take off immediately all contaminated clothing – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S9, S26, S27, S28, S45)

Ecotoxicity

Invertebrate toxicity

Not acutely toxic to freshwater benthic microbial communities, using acetate metabolism as the index of toxicity. Statistically significant effects were found in only 3/25 incubations and at trifluoroacetate concentrations much higher than measured to date in the environment or predicted from refrigerant sources: 175 nM in one experiment with WCC sediments, 17.5 µM in an experiment which indicated that a 16 hr preexposure of WCC sediments to trifluoroacetate did not significantly effect acetate metabolism, and 3859 µM in high exposure experiments (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 200 mg kg⁻¹ (2).

LC₅₀ inhalation rat 10 g m⁻³ (duration unspecified) (3).

LC₅₀ inhalation mouse 13,500 mg m⁻³ (duration unspecified) (3).

LD₅₀ intravenous mouse 1200 mg kg⁻¹ (4).

LD_{Lo} intraperitoneal mouse 150 mg kg⁻¹ (5).

Sub-acute and sub-chronic data

Induced hepatomegaly and peroxisome proliferation in rats administered 0.5% in their diet for 5-14 days (6).

Irritancy

Vapours are irritating to eyes and liquid may cause deep burns (species unspecified) (7).

Genotoxicity

Salmonella typhimurium TA98, TA100 with and without metabolic activation negative (8).

Predicted to be marginally genotoxic by a CASE structure-activity methodology (9).

Other effects

Other adverse effects (human)

In humans the major toxic effects of fluoroacetates involve the cardiovascular and central nervous systems. Inhalation may be fatal as a result of spasm, inflammation and oedema of the bronchi and larynx, chemical pneumonitis and pulmonary oedema. Symptoms may include a burning feeling, coughing, wheezing, laryngitis, dyspnoea, headache, nausea and vomiting (7).

Any other adverse effects

At >10⁻³M is non-toxic in rat Sertoli germ cell cultures (10).

Enlargement of the liver and effects on liver metabolism were seen in rats following treatment with trifluoroacetate (11).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (12).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (13).

References

1. Bott, T. L. et al *Bull. Environ. Contam. Toxicol.* 1998, **60**(3), 472-479.
2. Patty, F. A. (Ed.) *Industrial Hygiene and Toxicology* 2nd ed., Interscience Publishers, New York, NY, USA.
3. *Gig. Tr. Prof. Zabol.* 1966, **10**(3), 13.
4. *Ann. Med. Exp. Biol. Fenn.* 1968, **46**, 242.
5. *Toxicol. Appl. Pharmacol.* 1969, **15**, 83.
6. Just, W. W. et al *Hepatology (Baltimore)* 1989, **9**(4), 570-581.
7. *Chemical Safety Data Sheets* 1990, **3**, 277-279, The Royal Society of Chemistry, London, UK.

8. Waskell, L. *Mutat. Res.* 1978, **57**(2), 141-154.
9. Klopman, G. et al *Mutat. Res.* 1990, **228**, 1-50.
10. Lloyd, S. C. *Food Chem. Toxicol.* 1986, **24**(6-7), 653-654.
11. Stier, A. et al *Biochem. Pharmacol.* 1972, **21**(16), 2181-2192.
12. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
13. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T291 trifluoroacetic anhydride



$\text{C}_4\text{F}_6\text{O}_3$

Mol. Wt. 210.03

CAS Registry No. 407-25-0

Synonyms bis(trifluoroacetic) anhydride; hexafluoroacetic anhydride; perfluoroacetic anhydride; 2,2,2-trifluoroacetic anhydride; trifluoroacetyl anhydride

EINECS No. 206-982-9

RTECS No. AJ 9800000

Physical properties

M. Pt. -65°C B. Pt. $39-40^\circ\text{C}$ Specific gravity 1.487

Mammalian & avian toxicity

Irritancy

Dermal rabbit (24 hr) 500 mg caused severe irritation and 5 mg instilled into rabbit eye for 24 hr caused severe irritation (1).

References

1. Marhold, J. V. *Sbornik Vysledku Toxologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia

T292 trifluoromethane



CHF_3

Mol. Wt. 70.01

CAS Registry No. 75-46-7

Synonyms carbon trifluoride; Freon 23; R 23; fluoroform

EINECS No. 200-872-4

RTECS No. PB 6900000

Uses Refrigerant.

Physical properties

M. Pt. -160°C B. Pt. -84.4°C Specific gravity 1.935 (solid); 1.52 (liquid) at -100°C

Occupational exposure

UN No. 1984 HAZCHEM Code 2RE Conveyance classification non-flammable non-toxic gas

Other effects

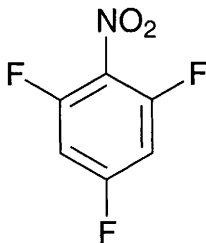
Any other adverse effects

Inhalation of 60% had no effect on cerebral blood flow, cerebral metabolic rate for O or oxyHb content in cats. At 70% the compound sensitised the cats' hearts to epinephrine and produced moderate changes in cerebral electrical activity (1).

References

1. Branch, C. A. et al *Stroke (Dallas)* 1990, **21**(8), 1172-1177

T293 2,4,6-trifluoronitrobenzene



$C_6H_2F_3NO_2$

Mol. Wt. 177.08

CAS Registry No. 315-14-0

Synonyms 1,3,5-trifluoro-2-nitrobenzene

EINECS No. 206-248-8

Physical properties

M. Pt. 3.5°C B. Pt. 182-185°C Flash point 77°C Specific gravity 1.514 at 20°C

Occupational exposure

UN No. 2306 HAZCHEM Code 2X Conveyance classification toxic substance

Ecotoxicity

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* concentration 134 mg l⁻¹; Microtox test (1).

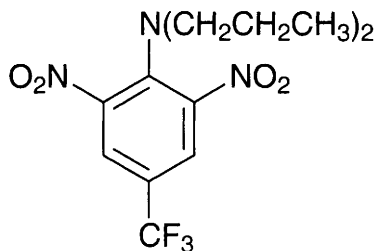
Legislation

Included in Schedule 4 (Release into Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (2).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
2. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T294 trifluralin



$C_{13}H_{16}F_3N_3O_4$

Mol. Wt. 335.28

CAS Registry No. 1582-09-8

Synonyms 2,6-dinitro-*N,N*-dipropyl-4-(trifluoromethyl)-benzenamine; α,α,α -trifluoro-2,6-dinitro-*N,N*-dipropyl-*p*-toluidine

EINECS No. 216-428-8

RTECS No. XU 9275000

Uses Selective herbicide.

Physical properties

M. Pt. 48.5-49.5°C (technical 43-47.5°C) **B. Pt.** 139-140°C at 4.2 mmHg **Partition coefficient** $\log P_{ow}$ 5.07 at pH 7 and 25°C (1) **Volatility** v.p. 2.0×10^{-4} mmHg at 29.5°C
Solubility Water: <1 mg l⁻¹ at 27°C. Organic solvents: acetone, xylene

Occupational exposure

Supply classification irritant

Risk phrases Irritating to the eyes – May cause sensitisation by skin contact (R36, R43)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with the skin – Wear suitable gloves (S2, S24, S37)

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) bluegill sunfish 19 µg l⁻¹ (2).
 LC₅₀ (48 hr) carp 1.0 mg l⁻¹ (3).
 LC₅₀ (96 hr) rainbow trout 0.21 mg l⁻¹ (4).
 LC₅₀ (96 hr) sheepshead minnow 0.19 mg l⁻¹ (5).
 LC₅₀ (96 hr) young rainbow trout, young bluegill sunfish 10-90 µg l⁻¹ (1).
 LOEC (chronic) fathead minnow 5 µg l⁻¹ (6).
 NOEC (chronic) fathead minnow 2 µg l⁻¹ (6).

Invertebrate toxicity

LC₅₀ (48 hr) *Daphnia magna*, *Asellus brevicaudus* 0.56, 0.2 mg l⁻¹, respectively (7).
 LC₅₀ (96 hr) *Procambarus clarkii* 12 mg l⁻¹ (8).
 NOEC *Daphnia magna* 3.5 µg l⁻¹ (6).
 EC₅₀ (10 day) *Chlorococcum* sp. 2.5 mg l⁻¹ (9).
 Oral toxicity to honeybees 0.011 mg bee⁻¹ (1).

Bioaccumulation

Bioconcentration factors in fish exposed to 1.8 µg l⁻¹: sauger 5800 (t_{1/2} 22-31 days); shorthead redhorse 2800 (t_{1/2} 17-57 days); golden redhorse 1800 (t_{1/2} 23 days); minnow sp. 6000 (t_{1/2} 3 days) (10).
 Estimated bioconcentration factors: mosquito fish 1294 (predicted from solubility correlation); rainbow trout 1030 (predicted from partition correlation) (10).

Environmental fate

Degradation studies

5 ppm degraded in non-sterile silt loam soil with <1% detected after 20 days at 25°C in the dark; anaerobic conditions maintained with N₂ (11).

Absorbed by soil and extremely resistant to leaching. Degradation occurs via dealkylation of the amino group, reduction of the nitro group to an amino group and partial oxidation of the trifluoromethyl group to a carboxy group. Duration of residual activity in soil is 6-8 months (1).

Soil t_{1/2} in irrigated soil: 3 wk in Texas; 5 wk in Tennessee (12,13).

Soil t_{1/2} in sandy loam soil under greenhouse conditions 50 days (14).

Soil t_{1/2} (initial concentration 750-1500 ppb) was 27.8-34.5 days in sandy soil and 32.3-35.6 days in loam (15).

Abiotic removal

Decomposed by UV irradiation (1).

Adsorption and retention

Trifluralin is moderately persistent and non-mobile in a microbially active soil environment (16).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 500, >10,000 mg kg⁻¹, respectively (1).

LD₅₀ oral dog, rabbit, chicken >2000 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

Dermal rabbit (14 day) 2 ml kg⁻¹ produced diarrhoea and slight erythema (17).

Oral rats (3 month) 0, 25, 50 or 100 mg kg⁻¹ day⁻¹ in the diet. No significant effects were observed on survival or appearance. Liver weights of animals fed 50 or 100 mg kg⁻¹ were increased compared with control animals (17).

Carcinogenicity and chronic effects

In 2-yr feeding trials, rats receiving 2000 mg kg⁻¹ diet and dogs receiving 1000 mg kg⁻¹ diet showed no ill-effects (1).

National Toxicology Program tested rats and mice via feed. No evidence of carcinogenicity was observed in ♂ and ♀ rats and ♂ mice. Positive evidence was observed in ♀ mice (18).

Oral mice (2 yr) 0, 75, 285 or 570 mg kg⁻¹ day⁻¹ in their diet. No treatment-related effects on the survival, appearance or behaviour were observed. Mean body weights of mice given 285 or 570 mg kg⁻¹ were reduced in a dose-related fashion compared with controls. Alanine aminotransferase activity was increased in all treated ♂ animals; blood urea nitrogen levels and alkaline phosphatase activity were increased in all mice receiving 285 or 570 mg kg⁻¹. A dose-related decrease in erythrocytic and leukocytic values was also seen at the two top concentrations. No increase in the incidence of benign or malignant neoplasms was observed in any mice (19).

Oral rats (2 yr) 0, 1, 10, 100 or 1000 mg kg⁻¹ day⁻¹ in their diet. No significant effects on growth rate, mortality or food consumption were seen at 1, 10 or 100 mg kg⁻¹. At 1000 mg kg⁻¹ animals were smaller than controls and had reduced food consumption (17).

Oral rats (2 yr) 30, 128 or 272 mg kg⁻¹ day⁻¹ for ♂ or 37, 54 or 336 mg kg⁻¹ day⁻¹ for ♀. A significant increase in malignant renal neoplasms and thyroid tumours in ♂ rats and in neoplasms of the bladder in both sexes was reported (dose level unspecified) (17).

Teratogenicity and reproductive effects

Gavage ♀ rabbits 0, 100, 225, 500 or 800 mg kg⁻¹ day⁻¹ during pregnancy. No adverse reproductive effects were seen at the two lower doses. Administration of 500 or 800 mg kg⁻¹ day⁻¹ resulted in anorexia, aborted litters and decreased live births (17).

Rabbits exposed to 225 or 500 mg kg⁻¹ day⁻¹ during pregnancy exhibited anorexia, cachexia and aborted litters. Decreased foetal size and weight were also observed at the highest dose (17).

Metabolism and toxicokinetics

Following oral administration in animals ~70% is eliminated in the urine and 15% in the faeces within 72 hr (1).

Irritancy

Non-irritating to rabbit skin (1).

Technical-grade trifluralin applied as a powder to rabbit eyes was non-irritating. Slight conjunctivitis developed but this cleared within a week. When applied as a 41.2% solution to rabbit eye, corneal opacity was produced which also cleared in 7 days (17).

Sensitisation

A 95% technical trifluralin solution was shown to be a potential skin sensitiser in guinea pigs using the Buehler topical-patch method (17).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA135, TA1537, TA1538 with and without metabolic activation negative (20).

In vitro L5178Y mouse lymphoma cells with and without metabolic activation negative (20).

In vivo Chinese hamster ovary cells with and without metabolic activation sister chromatid exchanges, chromosomal aberrations negative (20).

♀ Mice administered 1400 mg kg⁻¹ showed an increase in the number of micronuclei in the mouse bone marrow micronucleus test (21).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (22).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (23).

WHO Toxicity Class Table 5 (24).

EPA Toxicity Class III (acute dermal toxicity, inhalation toxicity and eye irritation potential), IV (acute oral toxicity and eye irritation potential) (16).

EEC Maximum Residue Limit – carrots, tomatoes, onions, artichokes, cabbages 0.05 ppm (1).

EPA tolerance for residues in/on wheat straw, barley straw, barley hay 0.1 ppm (16).

ADI 0.024 mg kg⁻¹ (25).

Other comments

Attributed endocrine disruption effects in wildlife. Fish vertebral anomalies (26).

Hazards reviewed (27).

Trifluralin adsorbed to sediment may pose a risk for fish species that forage by feeding from sediment, particularly since it has a moderate tendency to bioaccumulate (16).

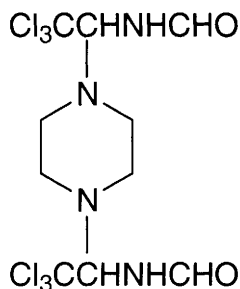
Metabolic pathways reviewed (28).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. Edwards, C. A. *Nature and Origins of Pollution of Aquatic Systems by Pesticides in Pesticides in Aquatic Environments* Khan, M. A. Q. (Ed.) 1977, Plenum Press, NY, USA.
3. Hashimoto, Y. et al *J. Pestic. Sci.* 1981, **6**, 257.
4. Macek, K. J. et al *Bull. Environ. Contam. Toxicol.* 1969, **4**, 174-183.
5. Parrish, P. R. et al *Chronic toxicity of chlordane, trifluralin, and pentachlorophenol to sheepshead minnows (Cyprinodon variegatus)* 1978, US EPA, Gulf Breeze, FL, EPA 600/3-78-010.
6. Macek, K. J. et al *Toxicity of four pesticides to water fleas and fathead minnows* 1976, US EPA, Duluth, MN, EPA 600/3-76-099.
7. Kenaga, E. E. *Down to Earth* 1979, **35**(2), 25-31.
8. Naqvi, S. M. et al *Bull. Environ. Contam. Toxicol.* 1983, **31**, 304-308.
9. Walsh, G. E. *Hyacinth Control J.* 1972, **10**, 45-48.
10. Spacie, A. et al *Environ. Sci. Technol.* 1979, **13**(7), 817-822.
11. Parr, J. F. et al *Soil Sci.* 1973, **115**(1), 55-63.
12. Menges, R. M. et al *Weed Sci.* 1980, **18**, 247.
13. Duseja, D. R. et al *Soil Sci.* 1978, **125**, 41.

14. Savage, K. E. *Weed Sci.* 1978, **26**, 465.
15. Zhang, D. et al *Shanghai Huanjing Kexue* 1988, **7**(6), 11-15 (Ch.) (*Chem. Abstr.* **110**, 71007h).
16. *Prevention, Pesticides and Toxic Substances (7508W)* April 1996, United States Environmental Protection Agency, EPA-738-F-95-035.
17. *Drinking Water Health Advisory – Pesticides* 1989, Lewis Publishers, Chelsea, MI, USA.
18. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-34, NIEHS, Research Triangle Park, NC, USA.
19. Francis, P. C. et al *Food Chem. Toxicol.* 1991, **29**(8), 549-555.
20. Garriott, M. L. et al *Mutat. Res.* 1991, **260**, 187-193.
21. Gebel, T. et al *Arch. Toxicol.* 1997, **71**(3), 193-197.
22. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
23. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; *6th Amendment EEC Directive* 79/831/EEC; *7th Amendment EEC Directive* 91/32/EEC 1991, HMSO, London, UK.
24. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
25. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
26. *Special Report on Environmental Endocrine Disruption: An Effects Assessment and Analysis* 1997, EPA/630/R-96/012, Risk Assessment Forum, US Environmental Agency, Washington, DC 20460, USA.
27. *Dangerous Prop. Ind. Mater. Rep.* 1990, **10**(2), 74-86.
28. Roberts, T. R. et al (Eds.) *Metabolic Pathways of Agrochemicals. Part 1: Herbicides and Plant Growth Regulators* 1998, The Royal Society of Chemistry, Cambridge, UK

T295 triforine



C₁₀H₁₄Cl₆N₄O₂

Mol. Wt. 434.96

CAS Registry No. 26644-46-2

Synonyms *N,N'*-[1,4-piperazinediylbis(2,2,2-trichloroethylidene)]bisformamide; biformylchlorazin; CELA 50; Funginex; Saprol; W 524

EINECS No. 247-872-0

RTECS No. TK 9200000

Uses Systemic fungicide.

Physical properties

M. Pt. 155°C (decomp.) **Partition coefficient** log *P*_{ow} 2.2 at 20°C (1) **Volatility** v.p. 2 × 10⁻⁷ mmHg at 25°C

Solubility Water: 9 mg l⁻¹ at 20°C. Organic solvents: dimethyl sulfoxide, *N*-methylpyrrolidinone, tetrahydrofuran

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bluegill sunfish, rainbow trout >1000 mg l⁻¹ (1).

Invertebrate toxicity

Not hazardous to bees at 600 mg l⁻¹ (2).

Environmental fate

Degradation studies

t_{1/2} in soil ~3 wk (1).

Abiotic removal

Decomposes in aqueous solution exposed to UV light or sunlight (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral bobwhite quail >5000 mg kg⁻¹ (1).

LD₅₀ oral rat, mouse, dog >16,000, >6000, >2000 mg kg⁻¹, respectively (1).

LC₅₀ (1 hr) inhalation rat >4.5 mg l⁻¹ (1).

LD₅₀ percutaneous rabbit, rat >10,000 mg kg⁻¹ (1).

LD₅₀ intraperitoneal rat >4000 mg kg⁻¹ (1).

Carcinogenicity and chronic effects

In a 2-yr feeding trial, no-effect level for rats was 625 mg kg⁻¹ diet, and for dogs 100 mg kg⁻¹ diet (1).

Genotoxicity

No increase in chromosomal aberrations was seen in workers spraying pesticides in closed spaces, however an increase was seen in workers exposed in open fields (3).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (4).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (5).

EEC Maximum Residue Limits – fruit and vegetables 1 ppm (1).

WHO Toxicity Class Table 5 (6).

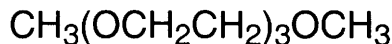
EPA Toxicity Class IV (2).

ADI (JMPR) 0.02 mg kg⁻¹ body weight (2).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
3. Nehez, M. et al *Regul. Toxicol. Pharmacol.* 1988, **8**(1), 37-44.
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
5. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
6. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21

T296 triglyme



$\text{C}_8\text{H}_{18}\text{O}_4$

Mol. Wt. 178.23

CAS Registry No. 112-49-2

Synonyms 2,5,8,11-tetraoxadodecane; triethylene glycol dimethyl ether; 1,2-bis(2-methoxyethoxy)ethane

EINECS No. 203-977-3

RTECS No. XF 0665000

Physical properties

M. Pt. -45°C B. Pt. 216°C Flash point 111°C Specific gravity 0.990 at 20°C with respect to water at 4°C
Solubility Water: miscible. Organic solvents: hydrocarbon solvents

Mammalian & avian toxicity

Teratogenicity and reproductive effects

In a preliminary developmental toxicity test, where pregnant mice were dosed orally on days 6-13 of gestation with 3.5 g kg^{-1} , the compound was found to be foetotoxic (1).

Similar results were found in mice following conventional tests (2).

Mice dosed orally on day 11 of pregnancy with 537 mg kg^{-1} showed no significant increase in malformations in foetus collected on day 18 (3).

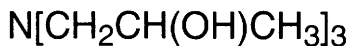
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (4).

References

1. Hardin, B. D. et al *Teratogen., Carcinogen., Mutagen.* 1987, 7, 29-48.
2. George, J. D. et al *Teratology* 1985, 31, 53A.
3. Hardin, B. D. *Teratology* 1987, 35(3), 321-328.
4. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T297 triisopropanolamine



$\text{C}_9\text{H}_{21}\text{NO}_3$

Mol. Wt. 191.27

CAS Registry No. 122-20-3

Synonyms tris(2-hydroxypropyl)amine; 1,1',1''-nitritoltri-2-propanol

EINECS No. 204-528-4

RTECS No. UB 8750000

Physical properties

M. Pt. $48-52^\circ\text{C}$ B. Pt. 190°C at 20 mmHg Flash point $>110^\circ\text{C}$ Specific gravity 1.02 at 20°C with respect to water at 20°C Volatility v.p. $<0.01 \text{ mmHg}$ at 20°C

Occupational exposure

Supply classification irritant

Risk phrases Irritating to the eyes (R36)

Safety phrases Keep out of reach of children (if sold to general public) – Wear suitable protective clothing (S2, S36)

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 2520, 6500 mg kg⁻¹, respectively (1,2).

LD_{Lo} dermal rabbit 10 g kg⁻¹ (3).

Irritancy

5 mg instilled into rabbit eye caused severe irritation (4).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (5).

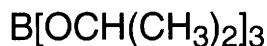
Other comments

Safe for use as cosmetic ingredient (6).

References

1. *Gig. Sanit.* 1980, 45(3), 79.
2. *J. Ind. Hyg. Toxicol.* 1948, 30, 63.
3. *Olin Chemicals Data Sheet* 1967, Olin Chemicals, New York, NY, USA.
4. *Am. J. Ophthalmol.* 1946, 29, 1363.
5. Zeiger, E. et al *Environ. Mol. Mutagen.* 1987, 9(Suppl. 9), 1-109.
6. Beyer, K. H. et al *Am. Coll. Toxicol.* 1987, 6(1), 53-76

T298 triisopropyl borate



C₉H₂₁BO₃

Mol. Wt. 188.07

CAS Registry No. 5419-55-6

Synonyms isopropyl borate; triisopropoxyborane

EINECS No. 226-529-9

RTECS No. ED 5950000

Physical properties

M. Pt. -59°C B. Pt. 139-141°C Flash point 10°C Specific gravity 0.8138 at 25°C

Occupational exposure

UN No. 2616 HAZCHEM Code 2ME Conveyance classification flammable liquid

Mammalian & avian toxicity

Acute data

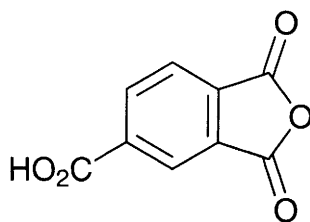
LD₅₀ oral, intravenous mouse 2500, 100 mg kg⁻¹, respectively (1,2).

Irritancy

100 mg instilled into rabbit eye caused mild irritation (1).

References

1. Adams, R. M. *Boron, Metallo-Boron Compounds and Boranes* 1964, John Wiley & Sons, New York, NY, USA.
2. NX 00382, U.S. Army Armament Research and Development Command, Chemical Systems Laboratory, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD, USA

T299 trimellitic anhydride

$C_9H_4O_5$

Mol. Wt. 192.13

CAS Registry No. 552-30-7

Synonyms 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid; 1,2,4-benzenetricarboxylic acid anhydride; 4-carboxyphthalic anhydride; NIC-C56633; TMA

EINECS No. 209-008-0

RTECS No. DC 2050000

Uses Preparation of resins, adhesives, polymers, dyes and printing inks.

Physical properties

M. Pt. 161-163.5°C B. Pt. 240-245°C at 14 mmHg Flash point 227°C Specific gravity 1.54 at 25°C

Volatility v.p. $<7 \times 10^{-9}$ mm Hg at 20°C; v.den. 6.6

Solubility Organic solvents: acetone, carbon tetrachloride, dimethylformamide, ethyl acetate, xylene

Occupational exposure

DE-MAK 0.04 mg m⁻³ (fume)

FR-VME 0.005 ppm (0.04 mg m⁻³)(fumes)

SE-LEVL 0.04 mg m⁻³

SE-CEIL 0.08 mg m⁻³

UK-LTEL 0.04 mg m⁻³

UK-STEL 0.12 mg m⁻³

US-STEL ceiling limit 0.04 mg m⁻³

UN No. 1693

Supply classification harmful

Risk phrases Irritating to the respiratory system – Risk of serious damage to eyes – May cause sensitisation by inhalation and skin contact (R37, R41, R42/43)

Safety phrases Keep out of reach of children (if sold to general public) – Do not breathe dust – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Wear suitable protective clothing, gloves and eye/face protection (S2, S22, S26, S36/37/39)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 5600 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

In a 90-day feeding study in rats and dogs, the no-effect level was 1000 and 20,000 ppm, respectively (2).

Inhalation rats 0-300 µg m⁻³ for varying durations. After 10 exposures for 6 hr day⁻¹, rats experienced external haemorrhagic lung foci, alveolar macrophage accumulation, alveolar haemorrhage, pneumonitis and lung and mediastinal lymph node damage. Rats exposed and rested 12 days were nearly recovered from these effects, but rats rested 12 days and subsequently challenged exhibited lesions similar to those seen immediately following exposure (3).

Other effects

Other adverse effects (human)

Three types of syndrome have been reported in workers exposed to fumes or dust during its manufacture. The first is a direct irritant response, with sneezing, occasional nose bleed, cough, laboured breathing and, rarely, wheezing which abates after 8 hours and rarely lasts into the night. The second, "TMA asthma" is rhinitis/asthma which develops after a sensitisation period of weeks or months. In the third, known as late onset respiratory systemic syndrome (LRSS) or "TMA flu", a sensitisation period of weeks or months is required and symptoms include wheezing, coughing, malaise, chills, fever and muscle and joint pains, and it is associated with relatively high levels of exposure. A fourth type of syndrome has been reported in workers exposed to fumes during the coating of hot pipes with epoxy resin containing trimellitic anhydride. It is severe and potentially fatal; effects include dyspnoea, pulmonary haemorrhages and haemolytic anaemia (4-6).

Any other adverse effects

Experiments in guinea pigs suggest that lung injury resulting from inhalation exposure to trimellitic anhydride can be induced with humoral antibodies and that at least two types of allergic reactions are involved in the pathogenesis of lung injury (7).

Other comments

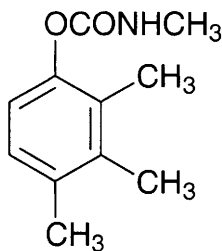
Hazards and precautions to be taken when used in the paint and ink industries reported (8).

Reviews on human health effects and experimental toxicology listed (9).

References

1. TLV's in Air, American Conference of Governmental Industrial Hygienists 1980, **4**, 415.
2. Toxicity Review 8, part 1: Trimellitic anhydride 1983, HMSO, London, UK.
3. Leach, C. L. et al *Toxicol. Appl. Pharmacol.* 1987, **87**(1), 67-80.
4. Zeiss, C. R. et al *J. Allergy Clin. Immunol.* 1977, **60**, 96.
5. Ahmed, D. et al *Lancet* 1979, **2**, 328.
6. AMOCO Chem. Corp. *Industrial Hygiene, Toxicology & Safety Data Sheet – Trimellitic anhydride* 1976, Med. & Health Serv. Dept.
7. Tao, Y. et al *Int. Arch. Allergy Appl. Immunol.* 1991, **96**(2), 119-127.
8. Scott, I.C. *J. Oil Colour Chem. Assoc.* 1986, **69**(11), 310-313.
9. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T300 2,3,4-trimethacarb



$C_{11}H_{15}NO_2$

Mol. Wt. 193.25

CAS Registry No. 3971-89-9

Synonyms 2,3,4-trimethylphenol methylcarbamate; methylcarbamic acid, 2,3,4-trimethylphenyl ester

RTECS No. FC 8400000

Uses Insecticide. Molluscicide.

Physical properties

M. Pt. 105-114°C **Volatility** v.p. 5.1×10^{-5} mmHg at 25°C

Environmental fate

Degradation studies

Soil $t_{1/2}$ ~60 days (1).

Legislation

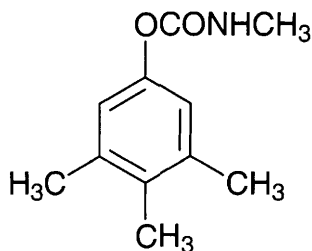
Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (2).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (3).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
3. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T301 3,4,5-trimethacarb



$C_{11}H_{15}NO_2$

Mol. Wt. 193.25

CAS Registry No. 2686-99-9

Synonyms 3,4,5-trimethylphenylmethylcarbamate

EINECS No. 220-245-9

RTECS No. FC 8575000

Uses Insecticide. Molluscicide.

Physical properties

M. Pt. 105-114°C Volatility v.p. 5.1×10^{-5} mmHg at 25°C

Solubility Water: >58 mg kg⁻¹ at 23°C. Organic solvents: not readily soluble in organic solvents.

Ecotoxicity

Fish toxicity

Toxic to fish (no details given) (1).

Environmental fate

Degradation studies

Soil $t_{1/2}$ ~60 days (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mallard duck, pigeon 22, 168 mg kg⁻¹, respectively (2).

LD₅₀ oral mouse, rat 101, 178 mg kg⁻¹, respectively (3,4).

LD₅₀ dermal rat >2000 mg kg⁻¹ (1).

LD_{Lo} intraperitoneal rat 136 mg kg⁻¹ (5).

LD₅₀ intravenous, intramuscular rat 32, 283 mg kg⁻¹, respectively (6).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (7).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (8).

Other comments

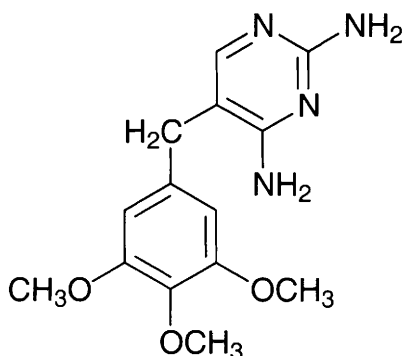
The commercial insecticide trimethacarb is a mixture of the 3,4,5- and 2,3,5-isomers (4:1 ratio).

In plants, metabolism occurs via hydroxylation of the *N*-methyl group and of the 3- and 4'-methyl positions. All metabolites may be conjugated as glucosides (1).

References

1. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
2. *Toxicol. Appl. Pharmacol.* 1971, **20**, 57.
3. *USDA Information Memorandum* 1966, Agric. Res. Serv., Beltsville, MD, USA.
4. *Toxicol. Appl. Pharmacol.* 1972, **21**, 315.
5. *Toxicol. Appl. Pharmacol.* 1973, **25**, 569.
6. *Br. J. Ind. Med.* 1965, **22**, 317.
7. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
8. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T302 trimethoprim



$C_{14}H_{18}N_4O_3$

Mol. Wt. 290.32

CAS Registry No. 738-70-5

Synonyms 5-[(3,4,5-trimethoxyphenyl)methyl]-2,4-pyrimidinediamine; 2,4-diamino-5-(3,4,5-trimethoxybenzyl)pyrimidine

EINECS No. 212-006-2

RTECS No. UV 8225000

Uses Antibiotic used to treat gastroenteritis, respiratory tract and urinary tract infections.

Physical properties

M. Pt. 199-203°C

Solubility Water: 0.04 g l⁻¹ at 20°C. Organic solvents: benzyl alcohol, chloroform

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 200, 3960 mg kg⁻¹, respectively (1,2).

LD₅₀ intraperitoneal mouse 1870 mg kg⁻¹ (3).

LD₅₀ intravenous mouse 200 mg kg⁻¹ (4).

Teratogenicity and reproductive effects

Virtually no effect on fertility reported in rats given 30 mg kg⁻¹ day⁻¹ subcutaneously for 6 wk (5).

Metabolism and toxicokinetics

In humans, rapidly and completely absorbed from the gastro-intestinal tract, peak plasma concentrations of 1 µg ml⁻¹ reported 1-4 hr after oral dose of 100 mg. 4.5% is bound to plasma proteins and it is widely distributed to various tissues and fluids. Readily crosses the placenta and appears in breast milk. t_{1/2} 8-11 hr. Excreted mainly

by kidneys. About 10-20% is metabolised in the liver and small amounts excreted in faeces via bile; 40-60% of a dose is excreted in urine within 24 hr (6).
Following intravenous administration of 25 mg kg⁻¹ to rats, elimination t_{1/2}, apparent volume of distribution in the central compartment and volume of distribution at steady state were 2059, 5729 and 2473 ml kg⁻¹, respectively; mean residence time, clearance and volume of distribution at steady state were 52 min, 40 ml min⁻¹ kg⁻¹ and 2097 ml, respectively. Tissue distribution was biphasic (7).

Irritancy

Pruritis and skin rash develop in 3 to 7% of patients treated (6).

Genotoxicity

Salmonella typhimurium TA98, TA1538 with and without metabolic activation positive (8).
Escherichia coli positive (metabolic activation unspecified) (9).

Other effects

Other adverse effects (human)

Most frequent adverse effects include pruritis and skin rash, and mild gastro-intestinal disturbances, including nausea, vomiting and sore mouth. Rarely, more severe skin reactions occur. Disturbances of liver enzymes values, increases in serum creatinine and blood-urea nitrogen levels, fever, hypersensitivity, anaphylaxis, and depression of haemopoiesis (observed as megaloblastic anaemia) and methaemoglobinemia have been reported (6).

Other comments

Toxicity and pharmacokinetics reviewed (10,11).
Side effects reviewed (12).

References

1. *International Congress of Chemotherapy* 1964, Proceedings of the 3rd Congress, Stuttgart, Germany.
2. *Kiso to Rinsho* 1979, **13**, 115.
3. *Chemotherapy* 1973, **21**, 175.
4. *Br. J. Pharmacol. Chemother.* 1968, **33**, 72.
5. Pholpramool, C. et al *Contraception* 1990, **42**(6), 667-675.
6. *Martindale. The Extra Pharmacopoeia* 30th ed., 1993, The Pharmaceutical Press, London, UK.
7. Tu, Y. H. et al *J. Pharm. Sci.* 1989, **78**(7), 556-560.
8. Rasool, S. A. et al *Mutat. Res.* 1987, **188**(3), 197-200.
9. Veigl, M. L. et al *Mutat. Res.* 1991, **246**(1), 75-91.
10. Corcoran, J. W. et al *Antibiotics* 1975, **3**, Springer-Verlag, New York, NY, USA.
11. Brogden, R. N. et al *Drugs* 1982, **23**, 405-430.
12. Francetic, I. *Pharmazie* 1986, **24**(3), 175-177 (Serbo-Croat.) (*Chem. Abstr.* **107**, 51216k)

T303 trimethylamine



C₃H₉N

Mol. Wt. 59.11

CAS Registry No. 75-50-3

Synonyms *N,N*-dimethylmethanamine; TMA

EINECS No. 200-875-0

RTECS No. PA 0350000

Uses In organic synthesis. Warning agent in natural gas. In manufacture of disinfectants. Flotation agent.

Occurrence Degradation product of nitrogenous plant and animal substances.

Physical properties

M. Pt. -117 to -124°C **B. Pt.** 2.87°C **Flash point** -6°C **Specific gravity** 0.662 at -5°C
Partition coefficient $\log P_{ow}$ 0.16 **Volatility** v.p. 1.44×10^3 mmHg; v.den. 2.0
Solubility Water: miscible. Organic solvents: benzene, chloroform, diethyl ether, toluene

Occupational exposure

FR-VLE 10 ppm (25 mg m⁻³)

UK-LTEL 10 ppm (25 mg m⁻³)

US-TWA 5 ppm (12 mg m⁻³)

UK-STEL 15 ppm (37 mg m⁻³)

US-STEL 15 ppm (36 mg m⁻³)

UN No. 1083 (anhydrous)

UN No. 1297 (aqueous solutions) **HAZCHEM Code** 2PE **Conveyance classification** flammable gas (anhydrous) **Conveyance classification** flammable liquid, corrosive (aqueous solutions)

Supply classification extremely flammable

Supply classification corrosive

Risk phrases Extremely flammable – Harmful by inhalation and if swallowed – Causes burns (R12, R20/22, R34)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep in a cool place – Keep away from sources of ignition – No smoking – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Do not empty into drains – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S3, S16, S26, S29, S36/37/39, S45)

Environmental fate

Nitrification inhibition

590 mg l⁻¹ caused 50% inhibition of ammonia oxidation (pure culture) (1).

118 mg l⁻¹ caused 75% inhibition of ammonia oxidation (activated sludge) (2).

Degradation studies

Batch tests indicate it can be metabolised at 1.18 g l⁻¹ by an aerobic, thermophilic microorganism isolated from fish meal processing gaseous effluent after acclimation (3).

Bacteria of the *Agrobacterium-Rhizobium* complex in rRNA superfamily IV use trimethylamine as a sole carbon and energy source (4).

Mammalian & avian toxicity

Acute data

LC_{Lo} (4 hr) inhalation rat 3500 ppm (5).

LD₅₀ intravenous mouse 90 mg kg⁻¹ (6).

LD_{Lo} subcutaneous rabbit 800 mg kg⁻¹ (7).

Sub-acute and sub-chronic data

Non-reversible degenerative changes in the nose and mild emphysematous alveoli reported in rats following nose-only inhalation of 750 ppm 6 hr day⁻¹, 5 day wk⁻¹ for 2 wk (8).

Teratogenicity and reproductive effects

Administration (route unspecified) of 0.174 mg kg⁻¹ to rats and mice was not foetotoxic (9).

Decreased foetal weight but not placental or maternal body weight reported in mice after intraperitoneal injection of 0.145-0.29 mg kg⁻¹ day⁻¹ on day 1-17 of pregnancy (10).

Metabolism and toxicokinetics

N-Oxidation was the major metabolic route in human volunteers after oral administration (11).

95% of 100 mg oral dose was excreted in urine of human volunteers within 24 hr (12).

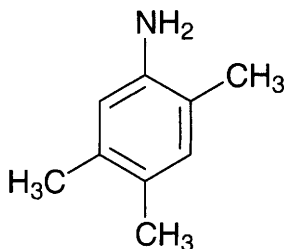
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (13).

References

1. Dickerson, D. W. *Sewage Ind. Wastes* 1950, **22**, 536.
2. Tomlinson, T. G. et al *J. Appl. Bacteriol.* 1966, **29**(2), 266-291.
3. Partidario, P. J. et al *Chem. Environ. Proc. Int. Conf.* 1986, 529-536.
4. Green, P. N. et al *J. Gen. Microbiol.* 1989, **135**(7), 2071-2076.
5. *Toxicology* 1984, **4**, 68.
6. *Med. Pharmacol. Exp.* 1967, **16**, 529.
7. *C. R. Seances Soc. Biol. Fil.* 1920, **83**, 481.
8. Kinney, L. A. et al *Inhalation Toxicol.* 1990, **2**(1), 41-51.
9. Varma, D. R. et al *J. Toxicol. Environ. Health* 1990, **30**(1), 1-14.
10. Guest, I. et al *J. Toxicol. Environ. Health* 1991, **32**(3), 319-330.
11. Al-Waiz, M. et al *Toxicology* 1987, **43**(2), 117-121.
12. Al-Waiz, M. et al *Xenobiotica* 1987, **17**(5), 551-558.
13. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T304 2,4,5-trimethylaniline



C₉H₁₃N

Mol. Wt. 135.21

CAS Registry No. 137-17-7

Synonyms 2,4,5-trimethylbenzenamine; ψ -cumidine; pseudocumidine; 1-amino-2,4,5-trimethylbenzene; 1,2,4-trimethyl-5-aminobenzene

EINECS No. 205-282-0

RTECS No. BZ 0520000

Uses Dyestuff synthesis.

Physical properties

M. Pt. 68°C **B. Pt.** 234-245°C **Specific gravity** 0.957 **Volatility** v.p. 1 mmHg at 68°C

Solubility Organic solvents: ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1250 mg kg⁻¹ (1).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, limited evidence for carcinogenicity to animals, IARC classification group 3 (2).

National Toxicology Program tested rats and mice via dosed-feed. Positive results for carcinogenicity in ♂ and ♀ rats and ♀ mice, equivocal results for ♂ mice (3).

Metabolism and toxicokinetics

In ♀ rats, haemoglobin bound covalently to 2,4,5-trimethylaniline at a binding index of 0.7. The haemoglobin adducts were hydrolysed under alkaline conditions (4).

Genotoxicity

Salmonella typhimurium TA98, TA100 with metabolic activation positive (5).

Drosophila melanogaster wing spot test positive for single small spots, negative for large single spots (6).

Chinese hamster ovary cells with and without metabolic activation induced sister chromatid exchange and without metabolic activation induced chromosomal aberrations (7).

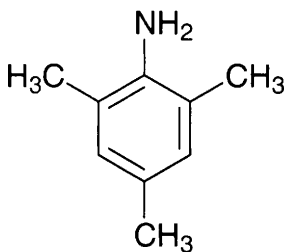
Other comments

Reviews on human health effects, experimental toxicology, epidemiology and workplace experience listed (8).

References

1. Sax, N. I. et al *Dangerous Properties of Industrial Materials* 8th ed., 1992, Van Nostrand Reinhold, New York, NY, USA.
2. IARC Monograph 1987, **Suppl. 7**, 73.
3. National Toxicology Program Research and Testing Division 1995, Report No. TR-160, NIEHS, Research Triangle Park, NC 27709, USA.
4. Birner, G. et al *Arch. Toxicol.* 1988, **62**(2-3), 110-115.
5. Zimmer, D. et al *Mutat. Res.* 1980, **77**, 317.
6. Kugler-Steigmeier, M. E. et al *Mutat. Res.* 1989, **211**(2), 279-289.
7. Loveday, K. S. et al *Environ. Mol. Mutagen.* 1990, **16**(4), 272-303.
8. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T305 2,4,6-trimethylaniline



C₉H₁₃N

Mol. Wt. 135.21

CAS Registry No. 88-05-1

Synonyms 2-aminomesitylene; aminomesitylene; 2,4,6-trimethylbenzenamine; mesidine; mesitylamine

EINECS No. 201-794-3

RTECS No. BZ 0700000

Uses Dyestuff synthesis.

Physical properties

M. Pt. -5°C B. Pt. 232-233°C Specific gravity 0.963

Occupational exposure

UN No. 2810

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 590, 740 mg kg⁻¹, respectively (1,2).

LC₅₀ (2 hr) inhalation mouse 290 mg m⁻³ (1).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (3).

Irritancy

Dermal rabbit (24 hr) 500 mg caused moderate irritation; 20 mg instilled into rabbit eye for 24 hr caused severe irritation (4).

Genotoxicity

Salmonella typhimurium TA98, TA100 with metabolic activation positive (5).

Drosophila melanogaster wing spot test positive for small single spots at higher concentrations, negative for large single spots (6).

Alkaline single cell gel electrophoresis (comet) assay in B6C3F1 mouse bone marrow cells positive (7).

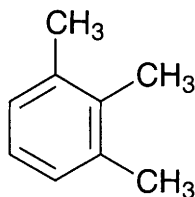
Other comments

Reviews on human health effects and experimental toxicology listed (8).

References

1. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, 20, Moscow, USSR.
2. Sax, N. I. et al *Dangerous Properties of Industrial Materials* 8th ed., 1989, Van Nostrand Reinhold, New York, NY, USA.
3. *IARC Monograph* 1987, **Suppl. 7**, 73.
4. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, 66, Prague, Czechoslovakia.
5. *Mutat. Res.* 1980, **77**, 317.
6. Kugler-Steigmeier, M. E. et al *Mutat. Res.* 1989, **211**(2), 279-289.
7. Przybojewska, B. *Mutat. Res.* 1997, **394**(1-3), 53-57.
8. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T306 1,2,3-trimethylbenzene



C₉H₁₂

Mol. Wt. 120.19

CAS Registry No. 526-73-8

Synonyms hemimellitene

EINECS No. 208-394-8

RTECS No. DC 3300000

Physical properties

M. Pt. -25.4°C B. Pt. 176.1°C Flash point 48°C Specific gravity 0.894 Partition coefficient $\log P_{ow}$ 3.66
Volatility v.den. 4.15

Occupational exposure

DE-MAK 20 ppm (100 mg m⁻³)

FR-VME 25 ppm (125 mg m⁻³)

JP-OEL 25 ppm (120 mg m⁻³)

SE-LEVL 25 ppm (120 mg m⁻³)

UK-LTEL 25 ppm (125 mg m⁻³)

US-TWA 25 ppm (123 mg m⁻³)

SE-STEL 35 ppm (170 mg m⁻³)

Ecotoxicity

Bioaccumulation

Non- or low accumulative (1).

Mammalian & avian toxicity

Acute data

LD_{Lo} oral rat 5000 mg kg⁻¹ (2).

Metabolism and toxicokinetics

Eight volunteers aged 20-39, with no history of exposure to trimethylbenzene, were exposed in 8 hr inhalation tests to 1,2,3-trimethylbenzene at concentrations ranging from 5 to 150 mg m⁻³. Pulmonary ventilation in the volunteers ranged from 0.56 to 1.0 m³ h⁻¹. The retention of 1,2,3-trimethylbenzene in the lungs was 71%. The highest rates of metabolic excretion and the highest quantities of dimethylbenzoic acids in the urine during 24-hr intervals were observed on day 5 of exposure (3).

Legislation

The $\log P_{ow}$ value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (4).

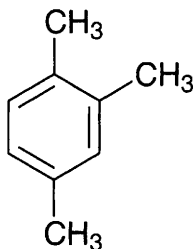
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (5).

References

1. *The list of the existing chemical substances tested on biodegradability by microorganisms or bioaccumulation in fish body* 1987, Chemicals Inspection & Testing Institute, Japan.
2. *Am. Med. Assoc. Arch. Ind. Health* 1959, **19**, 403.
3. Kostrzewski, P. et al *Sci. Total Environ.* 1997, **199**(1-2), 73-81.
4. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; *6th Amendment EEC Directive* 79/831/EEC; *7th Amendment EEC Directive* 91/32/EEC 1991, HMSO, London, UK.
5. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T307 1,2,4-trimethylbenzene



C₉H₁₂

Mol. Wt. 120.19

CAS Registry No. 95-63-6

Synonyms ψ-cumene; pseudocumol; asymmetrical trimethylbenzene; *as*-trimethylbenzene; 1,2,5-trimethylbenzene; pseudocumene

EINECS No. 202-436-9

RTECS No. DC 3325000

Uses In manufacture of trimellitic anhydride, dyes, pharmaceuticals and pseudocumidine.

Physical properties

M. Pt. -44°C **B. Pt.** 169°C **Flash point** 48°C **Specific gravity** 0.888 at 4°C with respect to water at 4°C
Partition coefficient log P_{ow} 3.78 **Volatility** v.p. 341 mm Hg at 140°C; v.den. 4.15
Solubility Water: 57 mg l⁻¹ at 20°C. Organic solvents: benzene, diethyl ether, ethanol

Occupational exposure

DE-MAK 20 ppm (100 mg m⁻³)

FR-VME 25 ppm (125 mg m⁻³)

JP-OEL 25 ppm (120 mg m⁻³)

SE-LEVL 25 ppm (120 mg m⁻³)

SE-STEL 35 ppm (170 mg m⁻³)

UK-LTEL 25 ppm (125 mg m⁻³)

US-TWA 25 ppm (123 mg m⁻³)

UN No. 2325 **HAZCHEM Code** 3 **Conveyance classification** flammable liquid

Supply classification harmful, dangerous for the environment

Risk phrases Flammable – Harmful by inhalation – Irritating to eyes, respiratory system and skin – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R10, R20, R36/37/38, R51/53)

Safety phrases Keep out of reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S26, S61)

Ecotoxicity

Invertebrate toxicity

EC₅₀ (48 hr) *Daphnia* spp. 0.03 mol m⁻³ (1).

LD₅₀ (24 hr) *Artemia* spp. 0.1 mol m⁻³ (1).

Bioaccumulation

Non- or low accumulative (2).

Environmental fate

Degradation studies

Degraded by isolates from well water and core material from a gasoline-contaminated shallow coastal aquifer containing *Pseudomonas*, *Alcaligenes*, *Nocardia* and *Micrococcus* (3).

Adsorption and retention

In a series of soils adsorption decreased in the order Gilat > Oxford > Bet Dagan. Adsorption on all soils was greater at 0% than 11.2% moisture. At 0% moisture, maximum adsorption on Oxford and Bet Dagan soils was $\sim 1000 \mu\text{g g}^{-1}$ at 20 days, and on Gilat soil was $\sim 4000 \mu\text{g g}^{-1}$ at 30 days. Bet Dagan is a red sandy clay (12% clay) with low organic matter content (0.5%); Gilat is a silty loam (16% clay) with low organic matter content (0.8%) and Oxford is a clay (35% clay) with 7.3% organic matter (4).

Mammalian & avian toxicity

Acute data

LC₅₀ (4 hr) inhalation rat 18 g m^{-3} (5).

LD_{Lo} intraperitoneal rat, guinea pig 1750, 1790 mg kg⁻¹, respectively (6,7).

Sub-acute and sub-chronic data

Inhalation rat 6 hr day⁻¹, 5 days wk⁻¹, for 4 wk at concentrations of 0, 25, 100, or 250 ppm. Results suggested that inhalation exposure to 1,2,4-trimethylbenzene may lead to long-lasting disturbances in CNS functions (8).

Metabolism and toxicokinetics

Brain/blood and fat/blood ratio was 2.0 and 63, respectively, in rats exposed to 1000 ppm (12 hr exposures; 14-day exposure period) (9).

Eight volunteers aged 20-39, with no history of exposure to trimethylbenzene, were exposed in 8-hr inhalation tests to 1,2,3-trimethylbenzene at concentrations ranging from 5 to 150 mg m⁻³. Pulmonary ventilation in the volunteers ranged from 0.56 to 1.0 m³ hr⁻¹. The retention of 1,2,3-trimethylbenzene in the lungs was 68%. The highest rates of metabolic excretion and the highest quantities of dimethylbenzoic acids in the urine during 24-hr intervals were observed on day 5 of exposure (10).

Legislation

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (11).

References

1. Abernethy, S. et al *Environ. Toxicol. Chem.* 1988, 7(6), 469-481.
2. *The list of the existing chemical substances tested on biodegradability by microorganisms or bioaccumulation in fish body* 1987, Chemicals Inspection & Testing Institute, Japan.
3. Reidgway, H. F. et al *Appl. Environ. Microbiol.* 1990, 56(1), 3565-3575.
4. Yaron, B. et al *J. Contam. Hydrol.* 1989, 4, 347-358.
5. *Gig. Sanit.* 1979, 4(5), 15.
6. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
7. *AMA Arch. Ind. Hyg. Occup. Med.* 1954, 9, 227.
8. Gralawicz, S. et al *Neurotoxicol. Teratol.* 1997, 19(4), 327-333.
9. Zahlsen, K. et al *Pharmacol. Toxicol. (Copenhagen)* 1990, 67(5), 436-440.
10. Kostrzewski, P. et al *Sci. Total Environ.* 1997, 199(1-2), 73-81.
11. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK

T308 trimethyl borate



$\text{C}_3\text{H}_9\text{BO}_3$

Mol. Wt. 103.91

CAS Registry No. 121-43-7

Synonyms borester; methyl borate; trimethyloxyborane; boric acid, trimethyl ester

EINECS No. 204-468-9

RTECS No. ED 5600000

Uses Solvent for waxes, resins and oils. Catalyst in ketone manufacture. In analysis of paint and varnish ingredients. Neutron detector in scintillation counter. Promoter of diborane reactions.

Physical properties

M. Pt. -34 to -29°C B. Pt. $68-69^\circ\text{C}$ Flash point -8°C Specific gravity 0.915 at 20°C Volatility v.den. 3.59

Solubility Organic solvents: miscible with diethyl ether, hexane, isopropylamine, methanol, tetrahydrofuran

Occupational exposure

UN No. 2416 HAZCHEM Code 2ME Conveyance classification flammable liquid

Supply classification harmful

Risk phrases Flammable – Harmful in contact with skin (R10, R21)

Safety phrases Keep out of reach of children (if sold to general public) – Do not breathe vapour – Avoid contact with the eyes (S2, S23, S25)

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 1290, 6140 mg kg⁻¹, respectively (1).

LD₅₀ dermal rabbit 1980 mg kg⁻¹ (2).

LD_{Lo} intraperitoneal mouse, rat 1000, 1600 mg kg⁻¹, respectively (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Boron: guide level 1000 µg l⁻¹ (3).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (4).

References

1. Adams, R. M. *Boron, Metallo-Boron Compounds and Boranes* 1964, John Wiley & Sons, New York, NY, USA.
2. *Am. Ind. Hyg. Assoc. J.* 1962, **23**, 95.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
4. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T309 trimethylene oxide



C₃H₆O

Mol. Wt. 58.08

CAS Registry No. 503-30-0

Synonyms 1,3-propylene oxide; cyclooxabutane; 1,3-epoxypropane; oxacyclobutane; α,γ -propane oxide; oxetane

EINECS No. 207-964-3

RTECS No. RQ 6825000

Physical properties

B. Pt. 48°C at 750 mmHg **Flash point** -28°C **Specific gravity** 0.8930 at 25°C with respect to water at 4°C

Occupational exposure

UN No. 1280 (blanketed with nitrogen) **HAZCHEM Code** 2WE (blanketed with nitrogen)

Conveyance classification flammable liquid (blanketed with nitrogen)

Supply classification highly flammable, harmful

Risk phrases Highly flammable – Harmful by inhalation, in contact with skin and if swallowed (R11, R20/21/22)

Safety phrases Keep out of reach of children (if sold to general public) – Keep container in a well ventilated place – Keep away from sources of ignition – No smoking – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Do not empty into drains (S2, S9, S16, S26, S29)

Mammalian & avian toxicity

Acute data

LD₅₀ subcutaneous rat 500 mg kg⁻¹ (1).

Genotoxicity

Salmonella typhimurium TA1535 with metabolic activation positive, TA97 with metabolic activation questionable mutagenic response (2).

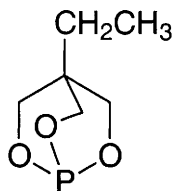
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (3).

References

1. *Z. Krebsforschung* 1970, **74**, 241.
2. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-158.
3. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T310 trimethylolpropane phosphite



$C_6H_{11}O_3P$

Mol. Wt. 162.13

CAS Registry No. 824-11-3

Synonyms 4-ethyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane; 2-ethyl-2-(hydroxymethyl)-1,3-propanediol, cyclic phosphite

EINECS No. 212-523-3

RTECS No. TY 6650000

Physical properties

M. Pt. 55-56°C B. Pt. 100°C at 8 mmHg

Mammalian & avian toxicity

Acute data

LD₅₀ oral dog, mouse, rat 5, 3, 8 mg kg⁻¹, respectively (1).

LD₅₀ intraperitoneal rat, mouse 1.02, 1.10 mg kg⁻¹, respectively (1,2).

LD₅₀ dermal rat 929 mg kg⁻¹ (1).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (3).

References

1. *Arch. Toxicol.* 1976, **35**, 149.
2. *Chem. Eng. News* 1974, **52**(1), 56.
3. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T311 trimethylolpropane triacrylate



$C_{15}H_{20}O_6$

Mol. Wt. 296.32

CAS Registry No. 15625-89-5

Synonyms 2,2'-bis(acryloyloxymethyl)butyl acrylate; TMPTA; 2-ethyl-2-(hydroxymethyl)-1,3-propanediol triacrylate; MFA (multifunctional acrylate); MFM (multifunctional monomer); 2-ethyl-2-[[[(1-oxo-2-propenyl)-oxy]methyl]-1,3-propanediyl] propenoate

EINECS No. 239-701-3

RTECS No. AT 4810000

Uses In radiation curing of urethanes, epoxy resins, and polyether resins. Manufacture of synthetic lubricants, coatings and ultra violet-cured inks.

Physical properties

M. Pt. <0°C **B. Pt.** >315.5°C **Flash point** >110°C (closed cup) **Specific gravity** 1.10 at 25°C with respect to water at 4°C **Volatility** v.p. <0.01 mmHg at 20°C

Occupational exposure

Supply classification irritant

Risk phrases Irritating to eyes and skin – May cause sensitisation by skin contact (R36/38, R43)

Safety phrases Keep out of reach of children (if sold to general public) – Wear eye/face protection (S2, S39)

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 5170-5190 mg kg⁻¹ (1,2).

LD₅₀ (24 hr) dermal rabbit 7000 mg kg⁻¹ (1).

Inhalation rat (6 hr) exposure to air saturated with bis(acryloyloxymethyl)butyl acrylate at 60°C caused no deaths (2).

Sub-acute and sub-chronic data

Dermal rabbits (2 wk) 500 mg kg⁻¹ day⁻¹ 5 day wk⁻¹ caused skin corrosion (2).

Carcinogenicity and chronic effects

Oral rats, mice 250-1000 ppm and 1250-2500 ppm, respectively, in food, induced hepatocellular carcinomas and haemangiosarcomas (3).

Positive correlation between hepatocarcinogenic effects in rats and binding of metabolites to liver DNA (4).

Selected for topical toxicology study in rats and mice by National Toxicology Program (5).

Irritancy

Dermal guinea pig, single application of 1-10% solution causes mild to moderate skin irritation. Single application of 0.1% solution, no reaction (6-8).

Sensitisation

Dermal guinea pig undiluted, no sensitisation in 10 animals (2).

Dermal guinea pig 1-5% solution, some sensitivity. Strong correlation between lymph node alterations and sensitisation potential (6).

Dermal guinea pigs caused no sensitisation on its own, but sensitised 6 out of 6 animals previously sensitised by other acrylates (7).

2,2'-Bis(acryloyloxymethyl)butyl acrylate caused contact hypersensitivity reactions in guinea pigs immunised with it in Freund's complete adjuvant. Cross-reactivity to pentaerythriol triacrylate, methyl acrylate, methyl vinyl ketone and 4-vinyl pyridine was reported (8).

Humans exposed to aerosols have developed dermatitis (3).

Genotoxicity

Salmonella typhimurium TA1535 with metabolic activation positive. Mouse lymphoma L5178Y tk⁺/tk⁻ assay without metabolic activation positive, with metabolic activation negative (9).

Induced mutations, aberrations and micronuclei in L5178Y mouse lymphoma cells without metabolic activation (10).

Other comments

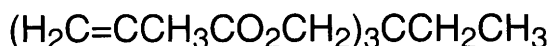
Reviews on human health effects and experimental toxicology listed (11).

References

1. Carpenter, C. P. et al *Toxicol. Appl. Pharmacol.* 1974, **28**, 313-319.
2. *Am. Ind. Hyg. Assoc. J.* 1981, **42**(11), B53-B54.

3. Emmet, E. A. et al *J. Occup. Med.* 1977, **19**(2), 113-115.
4. Bjoerkner, B. *Contact Dermatitis* 1984, **11**(4), 236-246.
5. *National Toxicology Program Research and Testing Div.* 1996, Management Status Report, NIEHS, Research Triangle Park, NC, USA.
6. Bull, J. E. et al *J. Invest. Dermatol.* 1985, **85**(5), 403-406.
7. Parker, D. et al *Contact Dermatitis* 1983, **9**(1), 55-60.
8. Parker, D. et al *Contact Dermatitis* 1985, **12**(3), 146-154.
9. Cameron, T. P. et al *Environ. Mol. Mutagen.* 1991, **17**(4), 264-271.
10. Dearfield, K. L. et al *Mutagenesis* 1989, **4**(5), 381-393.
11. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T312 trimethylolpropane trimethacrylate



C₁₈H₂₆O₆

Mol. Wt. 338.40

CAS Registry No. 3290-92-4

Synonyms TPT-MA; 2-ethyl-2-[[[(2-methyl-1-oxo-2-propenyl)oxy]methyl]-1,3-propanediyl 2-methyl-2-propenoate; 2-ethyl-2-hydroxymethyl-1,3-propanediol trimethacrylate; 2,2-bis[(methacryloyloxy)methyl]butyl methacrylate

EINECS No. 221-950-4

RTECS No. TY 6675000

Uses Manufacture of acrylic polymers, adhesives and cleaning agents. Cross-linking agent, vulcanisation agent and plasticiser. Polymer used in dental composites. Photoimaging materials.

Physical properties

M. Pt. -14°C **B. Pt.** 155°C at 1 mmHg **Flash point** >112°C (closed cup) **Specific gravity** 1.02 at 20°C with respect to water at 4°C **Partition coefficient** log P_{ow} 3.53

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal mouse 2889 mg kg⁻¹ (1).

Teratogenicity and reproductive effects

ED₅₀ (intraovary) 3-day-old white leghorn chick embryos 2.64 mg egg⁻¹ caused a maximum of 30% malformed embryos. LD₅₀ 4.4 mg egg⁻¹ caused early death (3-5 days after hatching) (2,3).

Sensitisation

Did not induce contact sensitisation reaction on guinea pig skin (4).

Genotoxicity

Salmonella typhimurium TA1535, with metabolic activation positive. Mouse lymphoma L5178Y without metabolic activation induced mutations, chromosome aberrations and micronuclei (5).

Mouse lymphoma L5178Y tk+ / tk- assay with or without metabolic activation negative (6).

Other comments

Reviews on human health effects and experimental toxicology listed (7).

References

1. Lawrence, W. H. et al *J. Dental Res.* 1972, **51**(2), 526-535.
2. Korhonen, A. et al *Scand. J. Work, Environ. Health* 1983, **9**(2), 115.
3. Korhonen, A. *Acta Pharmacol. Toxicol.* 1983, **52**(2), 95-99.
4. Parker, D. et al *Contact Dermatitis* 1983, **9**(1), 55-60.
5. Dearfield, K. L. et al *Mutagenesis* 1989, **4**(5), 381-393.
6. Cameron, T. P. et al *Environ. Mol. Mutagen.* 1991, **17**(4), 264-271.
7. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T313 trimethyl orthoformate



$\text{C}_4\text{H}_{10}\text{O}_3$

Mol. Wt. 106.12

CAS Registry No. 149-73-5

Synonyms methyl orthoformate; orthoformic acid, trimethyl ester; trimethoxymethane

EINECS No. 205-745-7

RTECS No. RM 6650000

Physical properties

B. Pt. 101-102°C Flash point 15°C Specific gravity 0.970 Volatility v.den. 3.67

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 3130 mg kg⁻¹ (1).

LC₅₀ (4 hr) inhalation rat 5000 ppm (1).

Irritancy

500 mg applied to rabbit skin caused mild irritation (1).

100 mg instilled into rabbit eye caused moderate irritation (1).

References

1. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia

T314 2,2,4-trimethylpentane



C_8H_{18}

Mol. Wt. 114.23

CAS Registry No. 540-84-1

Synonyms isooctane; isobutyltrimethylethane

EINECS No. 208-759-1

RTECS No. SA 3320000

Uses Organic synthesis. Solvent. In determining octane number of motor fuel. Spectrophotometric analysis.

Physical properties

M. Pt. -107.4°C **B. Pt.** 99.3°C **Flash point** -12°C (closed cup) **Specific gravity** 0.692 at 20°C with respect to water at 4°C **Volatility** v.p. 40.6 mmHg at 21°C; v.den. 3.93
Solubility Water: 0.56 mg l⁻¹ at 25°C. Organic solvents: benzene, carbon tetrachloride, chloroform, diethyl ether, toluene, xylene

Occupational exposure

UN No. 1262 **HAZCHEM Code** 3/E **Conveyance classification** flammable liquid

Environmental fate

Degradation studies

13% biodegradation of an initial concentration of 3.47 µl l⁻¹ after 192 hr at 13°C incubated with natural flora in groundwater in presence of other components of high octane petrol (1).

Degraded by *Pseudomonas putida*, *Pseudomonas stutzeri* and *Micrococcus* sp. isolated from contaminated well water (2).

Abiotic removal

t_{1/2} (calc.) in water at 25°C and 1 m depth 5.55 hr; evaporation rate 0.124 m hr⁻¹ (3).

Mammalian & avian toxicity

Metabolism and toxicokinetics

In rats exposed to 1 or 350 ppm radiolabelled ¹⁴C-isooctane for 2 hr, excretion was almost entirely via kidneys over the entire 70-hr post-exposure period. After this time 1-2% remained in the body (4).

Urinary metabolites in rats after oral administration included 1-hydroxy-2,3,4-trimethylpentane, 2,3,4-trimethyl-1-pentanoic acid and 2,3,4-trimethyl-5-hydroxy-1-pentanoic acid (5).

Irritancy

Eye irritation reactivity in humans 0.9 (6).

Other effects

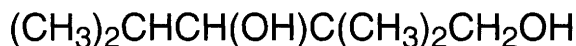
Any other adverse effects

Hepatotoxic as well as nephrotoxic in rats dosed with 2 ml kg⁻¹ in corn oil by gavage (7).

References

1. Jamison, V. W. et al *Proc. Third Int. Biodeg. Symp.* 1976, Applied Science Publishers, New York, NY, USA.
2. Ridgeway, H. F. et al *Appl. Environ. Microbiol.* 1990, **56**(11), 3565-3575.
3. Mackay, D. et al *Environ. Sci. Technol.* 1975, **9**(13), 1178-1180.
4. Dahl, A. R. *Toxicol. Appl. Pharmacol.* 1989, **100**(2), 334-341.
5. Olson, C. T. et al *Toxicol. Lett.* 1987, **37**(3), 199-202.
6. Yeung, C. K. K. et al *Atmos. Environ.* 1973, **7**, 551.
7. Fowlie, A. J. et al *J. Appl. Toxicol.* 1987, **7**(5), 335-341

T315 2,2,4-trimethyl-1,3-pentanediol



$\text{C}_8\text{H}_{18}\text{O}_2$

Mol. Wt. 146.23

CAS Registry No. 144-19-4

Synonyms TMPD (alcohol)

EINECS No. 205-619-1

RTECS No. SA 1400000

Uses Plasticiser in polyester resin used in food packaging.

Physical properties

M. Pt. 52-56°C B. Pt. 232°C at 4 mmHg Flash point >110°C

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 2000, 2200 mg kg⁻¹ respectively (1).

LD_{Lo} intraperitoneal rat, mouse 800 mg kg⁻¹ (2).

LD_{Lo} intravenous rat, mouse 145 mg kg⁻¹ (3).

Sub-acute and sub-chronic data

Oral (species unspecified) (60 day) 15 ♂ ♀ administered up to 2.0%. The ♀ ate less and gained less weight than controls and had a slight increase in average relative liver, adrenals, kidney, heart and brain weight. Haemograms and various enzyme activities were not affected (3).

Teratogenicity and reproductive effects

Oral (species unspecified) (60 day) 15 ♂ and 15 ♀ 1.0%, three-generation study, a decrease in pup weight was observed (3).

Irritancy

Repeated application to rabbit and guinea pig skin caused only slight to moderate erythema and moderate but transient irritation to rabbit eye (dose and duration unspecified) (3).

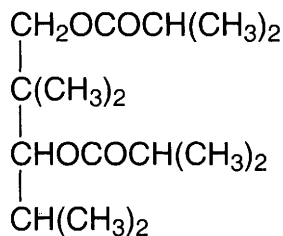
Other comments

Traces detected in water samples and mother's milk (4,2).

References

1. Sax's *Dangerous Properties of Industrial Materials* 8th ed., 1991, Van Nostrand Reinhold, New York, NY, USA.
2. Pellizzani, E. D. et al *Bull. Environ. Contam. Toxicol.* 1982, **28**, 322.
3. Terhaar, L. J. et al *Toxicol. Appl. Pharmacol.* 1974, **29**, 87.
4. Melton, R. G. et al *Identification and Analysis of Organic Pollutants in Water* Keith, L. H. (Ed.) 1982, **36**

T316 2,2,4-trimethyl-1,3-pentanediol diisobutyrate



$\text{C}_{16}\text{H}_{30}\text{O}_4$

Mol. Wt. 286.41

CAS Registry No. 6846-50-0

Synonyms 2,2,4-trimethyl-1,3-pentanediyl diisobutyrate; 2-methylpropanoic acid, 2,2-dimethyl-1-(1-methyl-ethyl)-1,3-propanediyl ester; 1-isopropyl-2,2-dimethyltrimethylene isobutyrate; C516; Kodaflex TXIB; Texanol isobutyrate

EINECS No. 229-934-9

RTECS No. SA 1420000

Physical properties

M. Pt. -70°C B. Pt. 280°C Flash point $>110^\circ\text{C}$ Specific gravity 0.941 Volatility v.den. 9.9

Mammalian & avian toxicity

Sub-acute and sub-chronic data

Oral σ and f albino rats 0.1 and 1.0% in diet for 52 day, 99 day, 52 day then a control diet for 47 day or fed a control diet for 52 day then the test diet for 47 day. An increase in relative liver weight, and increases in *p*-nitroanisoie demethylase, UDP-*p*-aminophenol and bilirubin glucuronyl transferase activities were observed. These changes occurred only in the animals fed the high-dose level and only when the animals were ingesting the compound at the time of sacrifice (1).

Intraperitoneal σ rats (7 day) 100 mg kg^{-1} . Elevated demethylase activity was observed when compared with the controls. No effect on the bilirubin glucuronyl transferase activity was noted (1).

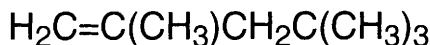
Irritancy

Dermal guinea pig 5 mg kg^{-1} caused mild irritation (duration unspecified) (2).

References

1. Krasavage, W. J. et al *Toxicol. Appl. Pharmacol.* 1972, 22(3), 400-408
2. *Toxicol. Appl. Pharmacol.* 1972, 22, 387.

T317 2,4,4-trimethylpentene



C_8H_{16}

Mol. Wt. 112.22

CAS Registry No. 25167-70-8

Synonyms diisobutene

EINECS No. 246-690-9

Uses Improving coatability in paper. Liquid laundry detergents.

Physical properties

B. Pt. 104-105°C Flash point >2°C (open cup) Specific gravity 0.724 at 15.5°C with respect to water at 15.5°C
Volatility v.p. 77.5 mmHg at 38°C; v.den. 4.9

Occupational exposure

UN No. 2050 HAZCHEM Code 3ME Conveyance classification flammable liquid

Supply classification highly flammable

Risk phrases Highly flammable (R11)

Safety phrases Keep out of reach of children (if sold to general public) – Keep container in a well ventilated place
– Keep away from sources of ignition – No smoking – Do not empty into drains – Take precautionary measures
against static discharges (S2, S9, S16, S29, S33)

Genotoxicity

Has been included in a CASE study to assess mutagenic potential (1).

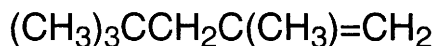
Other comments

Toxicology and human health effects reviewed (2,3).

References

1. Klopman, G. *Mutat. Res.* 1990, **228**(1), 1-50.
2. *Dangerous Prop. Ind. Mater. Rep.* 1981, **1**(8).
3. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T318 2,4,4-trimethyl-1-pentene



C₈H₁₆

Mol. Wt. 112.22

CAS Registry No. 107-39-1

Synonyms diisobutylene

EINECS No. 203-486-4

RTECS No. SB 2717300

Physical properties

M. Pt. -94°C B. Pt. 101-102°C Flash point 2°C (open cup) Specific gravity 0.708 Volatility v.den. 3.8

Occupational exposure

UN No. 2050 HAZCHEM Code 3ME Conveyance classification flammable liquid

Supply classification highly flammable, dangerous for the environment

Risk phrases Highly flammable – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R11, R51/53)

Safety phrases Keep out of reach of children (if sold to general public) – Keep container in a well ventilated place
– Keep away from sources of ignition – No smoking – Do not empty into drains – Take precautionary measures
against static discharges – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S9,
S16, S29, S33, S61)

Ecotoxicity

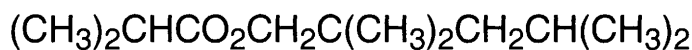
Fish toxicity

LC₅₀ (24 hr) goldfish 3 mg l⁻¹ (1).

References

1. *Environmental Properties of Chemicals. Research Report 91* 1990, Ministry of the Environment, VAPK-Publishing, Helsinki, Finland

T319 2,2,4-trimethylpentyl isobutyrate



C₁₂H₂₄O₂

Mol. Wt. 200.32

CAS Registry No. 36679-74-0

Synonyms 2,2,4-trimethylpentyl 2-methylpropionate; 2,2,4-trimethylpentyl 2-methylpropanoate

RTECS No. UA 2482000

Physical properties

B. Pt. 199-202°C at 747 mmHg Specific gravity 0.855 at 20°C

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 75 ml kg⁻¹ (toxic effects included ataxia and effects on the eyes and salivary glands) (1).

LD₅₀ dermal rabbit >16 ml kg⁻¹ (1).

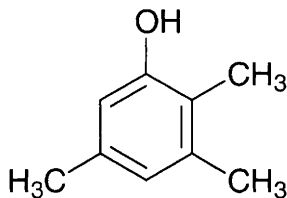
Irritancy

Dermal rabbit, 500 mg caused irritation. 100 mg instilled into rabbit eye caused irritation (exposure unspecified) (1).

References

1. *Acute Toxicity Data* 1992, 1, 193

T320 2,3,5-trimethylphenol



C₉H₁₂O

Mol. Wt. 136.19

CAS Registry No. 697-82-5

Synonyms 6-hydroxypseudocumene; isopseudocumenol

EINECS No. 211-806-9

Physical properties

M. Pt. 92-95°C B. Pt. 230-231°C

Ecotoxicity

Invertebrate toxicity

EC₅₀ (5 min) *Photobacterium phosphoreum* 9.64 ppm Microtox test (1).

Median inhibitory concentration (MIC) (24 hr) *Daphnia magna* 5.105 mmol l⁻¹ (2).

IC₅₀ (24 hr) *Daphnia magna* 0.196 mmol l⁻¹ (3).

IC₅₀ (24 hr) *Tetrahymena pyriformis* 8.51 mM (4).

Environmental fate

Degradation studies

Biodegradation by indigenous microorganisms from the American Creosote Works Superfund site, Pensacola, Florida. Initial concentration 0.4 µg ml⁻¹, after 14 days it was undetected (5,6).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phenols: maximum admissible concentration 0.5 µg l⁻¹ (7).

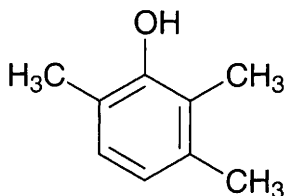
Other comments

A QSAR database study to determine the potential toxicity and risk to the environment from exposure to alkylphenols (8).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
2. Devillers, J. et al *Chemosphere* 1987, **16**(6), 1149-1163.
3. Devillers, J. et al *Sci. Total Environ.* 1988, **76**, 79-83.
4. Schultz, T. W. et al *Bull. Environ. Contam. Toxicol.* 1989, **43**, 192-198.
5. Mueller, J. G. et al *Appl. Environ. Microbiol.* 1991, **57**(5), 1277-1285.
6. Mueller, J. G. et al *Environ. Sci. Technol.* 1991, **25**, 1055-1061.
7. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
8. Beck, B. D. et al *Regul. Toxicol. Pharmacol.* 1991, **14**(3), 273-285.

T321 2,3,6-trimethylphenol



$C_9H_{12}O$

Mol. Wt. 136.19

CAS Registry No. 2416-94-6

Synonyms 3-hydroxypseudocumene

EINECS No. 219-330-3

Occurrence Present in tobacco smoke (1).

Physical properties

M. Pt. 62-64°C Partition coefficient $\log P_{ow}$ 2.67

Ecotoxicity

Invertebrate toxicity

EC₅₀ (5 min) *Photobacterium phosphoreum* 6.83 ppm Microtox test (2).

Environmental fate

Nitrification inhibition

At 4.9 mg l⁻¹ inhibition of nitrification, effect on V_{max} value (3).

At 17.2 mg l⁻¹ inhibition of nitrification, effect on K_m value (3).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phenols: maximum admissible concentration 0.5 µg l⁻¹ (4).

Other comments

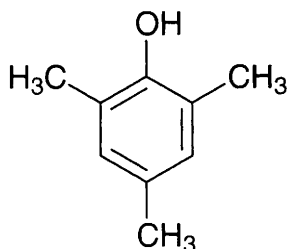
Reviews on human health effects, experimental toxicology, environmental effects, ecotoxicology and exposure levels listed (5).

A QSAR database study to determine the potential toxicity and risk to the environment from exposure to alkylphenols (6).

References

1. Arnarp, J. *Acta Chem. Scand.* 1991, **45**(5), 529-533.
2. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
3. Richardson, M. *Nitrification Inhibition in the Treatment of Sewage* 1985, The Royal Society of Chemistry, London, UK.
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
5. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
6. Beck, B. D. et al *Regul. Toxicol. Pharmacol.* 1991, **14**(3), 273-285

T322 2,4,6-trimethylphenol



C₉H₁₂O

Mol. Wt. 136.19

CAS Registry No. 527-60-6

Synonyms mesitol; 2-hydroxymesitylene; mesityl alcohol

EINECS No. 208-419-2

RTECS No. OX 6590000

Physical properties

M. Pt. 71-74°C B. Pt. 220°C Partition coefficient log P_{ow} 2.73

Ecotoxicity

Invertebrate toxicity

EC₅₀ (5 min) *Photobacterium phosphoreum* 11.9 ppm Microtox test (1).

EC₅₀ (24, 48 hr) *Daphnia magna* 5.7, 3.3 mg l⁻¹, respectively (2).

NOEC (21 day) *Daphnia magna* 34 mg l⁻¹ (3).

EC₅₀ (48 hr) *Scenedesmus subspicatus* 30 mg l⁻¹ (4).

IC₅₀ (24 hr) *Escherichia coli* 1.3 mmol l⁻¹ (5).

Median Inhibitory Concentration (MIC) (24 hr) *Escherichia coli* 2 mmol l⁻¹ (6).

Environmental fate

Nitrification inhibition

At 60.0 mg l⁻¹ inhibition of nitrification, effect on K_m value (7).

At 30.0 mg l⁻¹ inhibition of nitrification, effect on V_{max} value (7).

Degradation studies

Activated sewage sludge minimum degradation rate 1.9 g l⁻¹ hr⁻¹ (8).

Abiotic removal

Can be photodegraded (9).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phenols: maximum admissible concentration 0.5 µg l⁻¹ (10).

Other comments

A concentration of a 0.18 mg l⁻¹ was found in ground water at Gs Works Park, Seattle, WA (11).

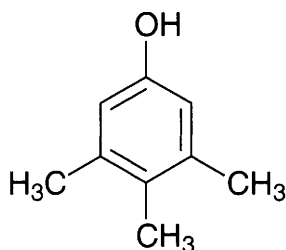
A QSAR database study to determine the potential toxicity and risk to the environment from exposure to alkylphenols (12).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, 26(3), 361-431.
2. Kuehn, R. et al *Water Res.* 1989, 23(4), 495-499.

3. Kuehn, R. et al *Water Res.* 1989, **23**(4), 501-510.
4. Kuehn, R. et al *Water Res.* 1990, **24**(1), 31-38.
5. Nendza, M. et al *Chemosphere* 1988, **17**(8), 1575-1584.
6. Nendza, M. et al *Ecotox. Environ. Saf.* 1990, **19**, 228-241.
7. Richardson, M. *Nitrification Inhibition in the Treatment of Sewage* 1985, The Royal Society of Chemistry, London, UK.
8. Stenstorm, M. K. et al *Environ. Prog.* 1989, **8**(2), 107-112.
9. Lin, K. et al *Mar. Chem.* 1991, **33**(1-2), 9-22.
10. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
11. Turney, G. L. et al *Ground Water Monit. Res.* 1990, **10**(3), 187-198.
12. Beck, B. D. et al *Regul. Toxicol. Pharmacol.* 1991, **14**(3), 273-285

T323 3,4,5-trimethylphenol



$C_9H_{12}O$

Mol. Wt. 136.19

CAS Registry No. 527-54-8

Synonyms 3,4,5-hemimellitenol

EINECS No. 208-418-7

Physical properties

M. Pt. 108-110°C

Ecotoxicity

Fish toxicity

IC₅₀ fathead minnow 8.51 mM l⁻¹ (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phenols: maximum admissible concentration 0.5 µg l⁻¹ (2).

Other comments

Detected in tobacco smoke (3).

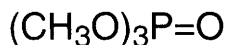
3,4,5-Trimethylphenol has antimycotic activity (4).

A QSAR database study to determine the potential toxicity and risk to the environment from exposure to alkylphenols (5).

References

1. Schultz, T. W. et al *Bull. Environ. Contam. Toxicol.* 1989, **43**, 192-198.
2. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
3. Arnarp, J. *Acta Chem. Scand.* 1991, **45**(5), 529-533.
4. Leifertova, I. et al *Folia. Pharm. (Prague)* 1988, **10**, 53-67.
5. Beck, B. D. et al *Regul. Toxicol. Pharmacol.* 1991, **14**(3), 273-285

T324 trimethyl phosphate



$\text{C}_3\text{H}_9\text{O}_4\text{P}$

Mol. Wt. 140.08

CAS Registry No. 512-56-1

Synonyms methyl phosphate; phosphoric acid, trimethyl ester; TMP; trimethyl orthophosphate

EINECS No. 208-144-8

RTECS No. TC 8225000

Uses Fuel additive for controlling surface ignition and spark plug fouling. Methylating agent. Catalyst in resin and polymer manufacture. Flame retardant in paints and polymers.

Physical properties

M. Pt. -46°C **B. Pt.** 197.2°C **Specific gravity** 1.197 at 19.5°C with respect to water at 0°C

Solubility Organic solvents: diethyl ether, ethanol

Ecotoxicity

Bioaccumulation

Non- or low accumulative (1).

Mammalian & avian toxicity

Acute data

LD_{50} oral rat, mouse 840, 1470 mg kg^{-1} , respectively (2).

LD_{50} oral rabbit 1050 mg kg^{-1} (3).

LD_{50} dermal rabbit 3388 mg kg^{-1} (4).

LD_{Lo} intraperitoneal, intravenous rat 800, 2400 mg kg^{-1} , respectively (5,6).

Sub-acute and sub-chronic data

Sedation and hind-limb paresis reported in rats treated 100 mg kg^{-1} $5 \times \text{wk}^{-1}$ for 1 yr (route unspecified) (7).

Carcinogenicity and chronic effects

National Toxicology Program tested mice and rats via gavage. Carcinogenic in σ rats and φ mice, not carcinogenic in φ rats and σ mice, (8).

It induced interuterine/endometrial adenocarcinomas in the φ mice and benign fibromas of the subcutaneous tissue in σ rats. Rats were dosed with 50-100 mg kg^{-1} and mice with 250-500 mg kg^{-1} , $3 \times \text{wk}^{-1}$ for 2 yr (8).

Oral σ and φ Wistar rats 0-100 mg kg^{-1} in drinking water for up to 30 months. Mortality was not affected in animals receiving up to 10 $\text{mg kg}^{-1} \text{ day}^{-1}$. Animals receiving 100 $\text{mg kg}^{-1} \text{ day}^{-1}$ had this dosage reduced by 50% in wk 54 and the animals were killed in wk 100. Animals of both sexes receiving the 100/50 mg kg^{-1} dose suffered weakness of the hindlimbs, increased incidences of sunken flanks, distended abdomen and poor general condition beginning with wk 46, and mortality reached around 70% by wk 100. The 100/50 mg kg^{-1} dose caused neurotoxic effects, consisting of degeneration and loss of nerve fibres in the peripheral nerves and spinal cord,

associated with myopathic changes. The no-observed-adverse-effect level (based on suppression of weight gain) was 1 mg kg⁻¹ for males and 10 mg kg⁻¹ for females. No indications of tumorigenic/carcinogenic effects were observed (9).

Teratogenicity and reproductive effects

Temporary sterility reported in ♂ rats administered 5 oral or intraperitoneal doses of 100-250 mg kg⁻¹ and mice administered 5 oral or intraperitoneal doses of 1 g kg⁻¹ (10).

Metabolism and toxicokinetics

Metabolised to dimethylphosphate, which is excreted in urine of rats and mice treated orally or intraperitoneally. Also metabolised to S-methylcysteine derivative and its N-acetate (11).

Genotoxicity

Salmonella typhimurium (strains and metabolic activation unspecified) positive (12).

Escherichia coli WP2 spot test positive (metabolic activation unspecified) (13).

Induced chromosome breaks in cultured human lymphocytes (metabolic activation unspecified) (14).

Induced chromatid aberrations *in vivo* in rats after intraperitoneal administration (metabolic activation unspecified) (15).

Micronucleus test in mice after intraperitoneal injection positive (16).

Induced dominant-lethal mutations in mice following a single intraperitoneal dose of 2000 mg kg⁻¹ or 5 oral doses of 500 mg kg⁻¹ (17,18).

Other comments

Genotoxicity reviewed (12).

References

1. *The list of the existing chemical substances tested on biodegradability by microorganisms or bioaccumulation in fish body* 1987, Chemicals Inspection & Testing Institute, Japan.
2. *Progress Report NIH-NCI-E-C-72-3252* 1973, Natl. Cancer Inst., Bethesda, MD, USA.
3. Deichmann, W. B. et al *J. Pharmacol. Exp. Ther* 1946, **88**, 338-342.
4. *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 470.
5. *J. Pharm. Pharmacol.* 1959, **11**, 150.
6. *Nature* 1957, **179**, 154.
7. Jones, A. R. et al *Br. J. Pharm.* 1969, **37**, 531-532.
8. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-81, NIEHS, Research Triangle Park, NC, USA.
9. Bomhard, E. M. et al *Fundam. Appl. Toxicol.* 1997, **40**(1), 75-89.
10. Jones, A. R. et al *Nature* 1968, **220**, 591-592.
11. Jones, A. R. et al *Experientia* 1970, **26**, 492-493.
12. Connor, T. H. *Mutat. Res.* 1979, **65**, 121-131.
13. Voogd, C. E. et al *Mutat. Res.* 1972, **16**, 413-416.
14. Soderman, G. et al *Hereditas* 1972, **71**, 335-338.
15. Adler, I. D. et al *Mutat. Res.* 1971, **13**, 263-273.
16. Weber, E. et al *Mutat. Res.* 1975, **28**, 101-106.
17. Epstein, S. S. et al *Science* 1970, **168**, 584-586.
18. Tezuka, H. et al *Mutat. Res.* 1985, **157**, 205-213.

T325 trimethyl phosphite



$\text{C}_3\text{H}_9\text{O}_3\text{P}$

Mol. Wt. 124.08

CAS Registry No. 121-45-9

Synonyms methyl phosphite; trimethyloxyphosphine; phosphorous acid, trimethyl ester

EINECS No. 204-471-5

RTECS No. TH 1400000

Uses In synthesis of organophosphates.

Physical properties

M. Pt. -78°C B. Pt. 111°C Flash point 27°C Specific gravity 1.046 at 20°C with respect to water at 4°C
Volatility v.den. 4.3

Occupational exposure

FR-VME 2 ppm (10 mg m^{-3})

UK-LTEL 2 ppm (10 mg m^{-3})

US-TWA 2 ppm (10 mg m^{-3})

UN No. 2329 HAZCHEM Code 3Y Conveyance classification flammable liquid

Mammalian & avian toxicity

Acute data

LD_{50} oral rat 1600 mg kg^{-1} (1).

LD_{Lo} dermal rabbit 2200 mg kg^{-1} (2).

LD_{50} intraperitoneal mouse 4180 mg kg^{-1} (3).

Teratogenicity and reproductive effects

Gross foetal abnormalities, skeletal defects, soft tissue defects and increased resorptions reported in rats administered $164\text{ mg kg}^{-1}\text{ day}^{-1}$ (but not 16 or $49\text{ mg kg}^{-1}\text{ day}^{-1}$) by gavage on days 6-15 of pregnancy (4).

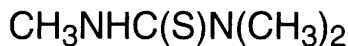
Irritancy

100 mg instilled into rabbit eye, or 500 mg applied to rabbit skin caused severe irritation (2).

References

1. OPB-3, 1984, Albright & Wilson, Richmond, VA, USA.
2. Deichmann, W. P. *Toxicology of Drugs and Chemicals* 1969, Academic Press, New York, NY, USA.
3. *Environ. Res.* 1975, 9, 1.
4. Mehlman, M. A. et al *Toxicol. Appl. Pharmacol.* 1984, 72, 119-123

T326 trimethylthiourea



$\text{C}_4\text{H}_{10}\text{N}_2\text{S}$

Mol. Wt. 118.20

CAS Registry No. 2489-77-2

Synonyms urea, 1,1,3-trimethyl-2-thio-; thiate E

EINECS No. 219-644-0

RTECS No. YU 4900000

Physical properties

M. Pt. 81-82°C

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 215, 316 mg kg⁻¹, respectively (1).

Carcinogenicity and chronic effects

Tumour found in thyroid gland of ♀ rat only, in tests on ♂ and ♀ rats and mice. Doses applied were 500 and 250 ppm for rats and 1000 and 500 ppm for mice (108 wk) (2-5).

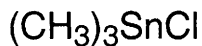
Genotoxicity

Salmonella typhimurium (type and metabolic activation unspecified) negative. *In vitro* Chinese hamster ovary cells mutagenic. *In vitro* Chinese hamster ovary cells sister chromatid exchanges negative (metabolic activation unspecified) (2,3).

References

1. Progress Report for contract no. NIH-NCI-E-C0-72-3252, Submitted to the National Cancer Institute by Litton Biometric Inc., Bethesda, MD, USA.
2. Rosenkranz, H. S. et al *Mutagenesis* 1990, 5(6), 559-571.
3. Zeiger, E. et al *Cancer Res.* 1987, 47, 1287-1296.
4. Benigni, R. *Mutat. Res.* 1990, 244, 79-91.
5. National Toxicology Program Research and Testing Division 1992, Report No. TR-129, NIEHS, Research Triangle Park, NC, USA

T327 trimethyltin chloride



$\text{C}_3\text{H}_9\text{ClSn}$

Mol. Wt. 199.27

CAS Registry No. 1066-45-1

Synonyms chlorotrimethyl-stannane; M & T Chemicals 1222-45; trimethylchlorotin; trimethylstannyl chloride

EINECS No. 213-917-8

RTECS No. WH 6850000

Physical properties

M. Pt. 37°C Flash point 97°C

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Sn) (total dust)

SE-LEVL 0.1 mg m⁻³ (as Sn)

SE-STEL 0.2 mg m⁻³ (as Sn)

UK-LTEL 0.1 mg m⁻³ (as Sn)

UK-STEL 0.2 mg m⁻³ (as Sn)

US-TWA 0.1 mg m⁻³ (as Sn)

US-STEL 0.2 mg m⁻³ (as Sn)

UN No. 2788 (liquid)

UN No. 3146 (solid) HAZCHEM Code 2X (solid) Conveyance classification toxic substance

Supply classification very toxic

Risk phrases Very toxic by inhalation, in contact with skin and if swallowed (R26/27/28)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Take off immediately all contaminated clothing – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S26, S27, S28, S45)

Ecotoxicity

Invertebrate toxicity

EC₅₀ *Skeletonema costatum* 214 µg l⁻¹ (calculated) (1).

EC₅₀ *Thalassiosira pseudonana* 348 µg l⁻¹ (calculated) (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird 98 mg kg⁻¹ (2).

LD₅₀ oral rat 12.6 mg kg⁻¹ (3).

LD₅₀ intraperitoneal rat 7450 µg kg⁻¹ (4).

LD₅₀ intravenous mouse 1800 µg kg⁻¹ (5).

Metabolism and toxicokinetics

Intraperitoneal rats 7 mg kg⁻¹ of [¹⁴C]TMT on days 12 or 17 of gestation. Radioactivity in gestation days 12 and 17 maternal whole blood peaked after 1 hr. Whole blood elimination half-lives were 12-15 days. Combined urinary and faecal elimination of radiolabel for 2 wk after dosing accounted for 31 and 2% of the gestation day 12 and 17 doses, respectively (6).

Genotoxicity

In vitro human peripheral blood lymphocytes of ♂ and ♀ 0.5 µg and 1.0 µg, respectively. A significant increase in micronucleus counts increased frequencies of abnormal cells and chromosomal aberrations were observed (7).

Other effects

Any other adverse effects

Intraperitoneal rats, tin accumulated in the brain and behavioural abnormalities such as aggression and hyperactivity were encountered, a decrease in noradrenalin was also observed. Changes in acetylcholine levels occurred in the late stages and correlated with the proliferation of astrocytes and necrosis of neurons (8).

In vitro isolated rat hepatocytes at 1-100 µg ml⁻¹ for 2 hr caused a rapid decrease in cell viability (9).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (10).

Other comments

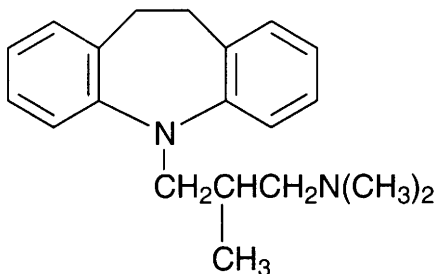
Reviews on human health effects, experimental toxicology, environmental effects, ecotoxicology, exposure levels and hazard assessment listed (11).

Organotins (unspecified) enhanced the induction of chromatid aberrations by clastogenic pollutants in chlorinated tap water, indicating a potential increased risk to health (12).

References

1. Walsh, G. E. et al *Environ. Toxicol. Chem.* 1987, **6**, 767-770.
2. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 35-382.
3. *Am. J. Pathol.* 1979, **97**, 59.
4. *Neurobehavioural Toxicol.* 1982, **4**, 127.
5. Report NX 09283, US Army Armament Research and Development Command, Chemical Systems Laboratory, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD, USA.
6. Lipscomb, J. C. et al *Neurotoxicol. Teratol.* 1989, **11**(2), 185-191.
7. Ghosh, B. B. et al *Mutat. Res.* 1990, **245**(1), 33-39.
8. Noguchi, Y. *Nichidai Igaku Zasshi* 1990, **49**(12), 1219-1228.
9. Yamada, J. *Agric. Biol. Chem.* 1991, **55**(9), 2313-2319.
10. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
11. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
12. Sasaki, Y. F. et al *Mutat. Res.* 1993, **300**(1), 5-14

T328 trimipramine



C₂₀H₂₆N₂

Mol. Wt. 294.44

CAS Registry No. 739-71-9

Synonyms 10,11-dihydro-*N,N*,β-trimethyl-5*H*-dibenz[*b,f*]azepine-5-propanamine; IL6001; β-methylimipramine; Sapilent; surmontil; trimeproprimine

EINECS No. 212-008-3

RTECS No. HO 1225000

Uses Antidepressant.

Physical properties

M. Pt. 45°C

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 250 mg kg⁻¹ (1).

LD₅₀ intraperitoneal mouse 145 mg kg⁻¹ (2).

LD₅₀ subcutaneous mouse 200 mg kg⁻¹ (1).

LD₅₀ intravenous mouse 42 mg kg⁻¹ (2).

Metabolism and toxicokinetics

The following metabolites were identified in man: mono- and dihydroxy-trimipramine; hydroxymethoxytrimipramine; iminodibenzyl; mono- and dihydroxy-iminodibenzyl; hydroxymethoxy-iminodibenzyl; nor-T(NT); mono- and dihydroxy-NT; hydroxymethoxy-NT; bis-nor-T(BNT); mono- and dihydroxy-BNT and hydroxymethoxy-BNT (3).

Other effects

Other adverse effects (human)

It has been stated to delay or inhibit ejaculation (4).

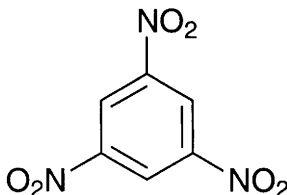
Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (5).

References

1. *Boll. Chim. Farm.* 1963, **102**, 753.
2. *C. R. Seances Soc. Biol. Ses Fil.* 1961, **155**, 307.
3. Maurer, H. *Arzneim.-Forsch.* 1989, **39**(1), 101-103.
4. Beeley, L. *Adverse Drug React. Acute Poisoning Rev.* 1984, **3**, 23-42.
5. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T329 1,3,5-trinitrobenzene



C₆H₃N₃O₆

Mol. Wt. 213.11

CAS Registry No. 99-35-4

Synonyms TNB; s-trinitrobenzene

EINECS No. 202-752-7

RTECS No. DC 3850000

Uses Explosive, less sensitive to impact than TNT but more powerful.

Physical properties

M. Pt. 122°C B. Pt. decomp. Specific gravity 1.760 at 20°C with respect to water at 4°C

Solubility Water: 350 mg l⁻¹. Organic solvents: acetone, benzene, carbon disulfide, diethyl ether, ethanol, methanol, light petroleum

Occupational exposure

UN No. 1354 Conveyance classification flammable solid

Supply classification explosive, very toxic

Risk phrases Risk of explosion by shock, friction, fire or other sources of ignition – Very toxic by inhalation, in contact with skin and if swallowed – Danger of cumulative effects (R2, R26/27/28, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – This material and its container must be disposed of in a safe way – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S35, S45)

Ecotoxicity

Fish toxicity

Administration of 0.13-0.61 mg l⁻¹ to bluegill sunfish caused significant changes in ventilatory depth respiration and body movement (1).

LC₅₀ (96 hr) fathead minnow 1.03 mg l⁻¹ (2).

Invertebrate toxicity

EC₅₀ (48 hr) *Daphnia magna* 3 mg l⁻¹ (2).

EC₅₀ (30 min) *Vibrio fischeri* 0.20 mg l⁻¹ (3).

Bioaccumulation

Estimated bioconcentration factors 5 and 23 based on a log P_{ow} of 1.18 and a water solubility of 340 mg l⁻¹ at 20°C, respectively, which suggest accumulation is insignificant in aquatic organisms (4,5).

Environmental fate

Degradation studies

Transformation of 0.5 mM, incubated for 30 day with methanogenic bacteria, *Methanococcus* sp. (strain B) 100%, *M. deltae* 70%, *M. thermolithotrophicus* 65% (6).

Microbial degradation was incomplete and unsustained in Tennessee river water. Nitro group reduction occurred in the presence of added nutrients and laboratory cultures of Tennessee river microorganisms (7).

At an initial concentration of 100 ppm, 1,3,5-trinitrobenzene was found to be resistant to biodegradation when incubated 180 minutes in a phenol-adapted mixed culture of microorganisms obtained from garden soil, compost, river sediment and a petroleum refinery waste lagoon (8).

Abiotic removal

Chromophores absorb ultraviolet light at >290 nm, which suggests potential hydrolysis when exposed to sunlight (9).

Estimated photochemical t_{1/2} 35 yr (10).

Volatilisation from water is not expected to be an environmentally important fate process (4).

Adsorption and retention

Estimated soil adsorption coefficients of 104 and 178 suggest moderate to high mobility in soil and moderate to low adsorption by suspended solids and sediments in water (4,5,11).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat, guinea pig 280-730 mg kg⁻¹ (12-14).

LD₅₀ intravenous mouse 32 mg kg⁻¹ (15).

Sub-acute and sub-chronic data

♂ and ♀ Rats were exposed to 0, 50, 200, 400, 800 and 1200 mg kg⁻¹ chow diet for 14 days. Food intake was reduced and resulted in significant decreases in absolute weight in both sexes exposed to 800 and 1200 mg TNB kg⁻¹ diet and in ♀ rats exposed to 400 mg TNB kg⁻¹ diet. An increase in spleen weight of both sexes in high-dose groups occurred and the kidney, spleen, brain and testes were susceptible to TNB toxicity. ED_{Lo} 4.41 mg TNB body weight⁻¹ day⁻¹ (16).

Teratogenicity and reproductive effects

♂ and ♀ Sprague-Dawley rats were fed 30, 150 or 300 mg kg⁻¹ over 90 days, resulting in a decrease in mean body-weight in both sexes of high-dose rats. Sperm depletion and degeneration of the seminiferous tubules were noted, and methaemoglobinemia and splenic haemosiderosis were common in the high-dose and mid-dose rats of both sexes at necropsy (17).

Male rats were exposed to 0-1200 mg 1,3,5-trinitrobenzene kg⁻¹ chow diet for 14 days. High-dose animals suffered a decrease in testicular weight (16).

Irritancy

Dermal rabbit (24 hr) 0.5g caused no skin irritation. 0.1g applied to rabbit eyes caused severe irritation, and irreversible damage to ocular tissues. Considered to be corrosive (18).

Skin irritant characterised by hyperaemia, oedema and haemorrhages in experimental animals (14).

Sensitisation

Guinea pigs exposed to 1,3,5-trinitrobenzene once a week for 3 weeks, then challenged in week 5 for 24 hr, showed mild skin sensitisation (18).

Genotoxicity

Salmonella typhimurium TA1535, TA1537, TA1538, TA98, TA100 with and without metabolic activation positive (19).

Other effects

Any other adverse effects

A single oral dose of 85 mg kg⁻¹ to rat caused 50% methaemoglobinaemia (20).

Legislation

Included in the UK List of Classified and Authorised Explosives 1994. UK Class and Division 3.2. Competent Authority Reference S 13/680/91 (21).

Other comments

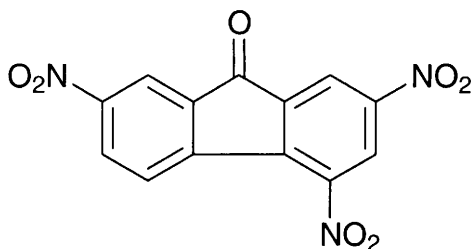
General literature review of aromatic amino and nitro compounds (22).

Reviews on human health effects, experimental toxicology and environmental effects listed (23).

References

1. Van der Schalie, W. H. *Aquatic Toxicol. Hazard Assess.* 1988, **10**, 307-3152.
2. Pearson, J. G. et al *Aquatic Toxicology* 1979, 284-301, ASTM STP 667.
3. Drzyzga, O. et al *Arch. Environ. Contam. Toxicol.* 1995, **28**(2), 229-235.
4. Lyman, W. J. et al *Handbook of Chemical Property Estimation Methods* 1982, McGraw-Hill, New York, NY, USA.
5. Hansch, C. et al *Medchem Project* 1985, 25, Pomona College, Claremont, CA, USA.
6. Boopathy, R. *Arch. Microbiol.* 1994, **162**(3), 167-172.
7. Mitchell, W. R. et al *Report* 1982, Iss USAMBRDL- TR-8201, AD-A116651.
8. Tabak, H. H. et al *J. Bacteriol.* 1964, **87**, 910-919.
9. Mill, T. et al *Environmental Exposure from Chemicals* 1985, **1**, CRC Press, Boca Raton, FL, USA.
10. Atkinson, R. *Int. J. Chem. Kinet.* 1987, **19**, 799-828.
11. Swann, R. L. et al *Res. Rev.* 1983, **85**, 17-28.
12. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, 117, Moscow, USSR.
13. *Gig. Sanit.* 1977, **42**(10), 12-77, (Russ).
14. Timatievskaya, L. A. *Toxicol. New Ind. Chem. Subst.* 1973, **13**, 138-133 (Russ.).
15. *US Army Armament Research and Development Command* NX00192.
16. Reddy, T. V. et al *J. Appl. Toxicol.* 1996, **16**(4), 289-295.
17. Kinkad, E. R. et al *Toxicol. Ind. Health* 1995, **11**(3), 309-323.
18. Fitzgerald, G. B. et al *Acute Toxic. Data* 1992, **1**(3), 169-170.
19. McGregor, D. B. et al *Environ. Mol. Mutagen.* 1980, **2**(4), 531-541.
20. Senczuk, W. et al *Bromatologica i Chemia Totsykologiczna* 1976, **9**(3), 289-294 (Pol.).
21. *UK Explosives Acts, 1975 and 1923. The Classification and Labelling of Explosives Regulations* 1983 (CLER). *List of Classified and Authorised Explosives* 1994 (LOCAE) 1994, HSE, UK.
22. Von-Oettingen, W. F. *Public Health Bull.* 1941, **271**, 1-228.
23. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T330 2,4,7-trinitrofluorenone



$C_{13}H_5N_3O_7$

Mol. Wt. 315.20

CAS Registry No. 129-79-3

Synonyms 2,4,7-trinitro-3*H*-fluoren-9-one; TNF

EINECS No. 204-965-0

RTECS No. LL 9100000

Uses In photocopiers. Forms charge-transfer complexes with aromatic hydrocarbons and amines.

Physical properties

M. Pt. 175-176°C

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 9910 mg kg⁻¹ (1).

Teratogenicity and reproductive effects

Oral mouse 3000 mg kg⁻¹ day⁻¹ on gestation days 8-12, no effects to mother or litter observed (2).

Irritancy

Dermal rabbit (24 hr) 300 mg caused mild irritation and 100 mg instilled into rabbit eye caused mild irritation (3).

Genotoxicity

It was cytotoxic to human teratocarcinoma (PA1) cells, mouse Sertoli (TM4) cells, rat hepatoma (RL-12) cells human - Chinese hamster ovary cells (CHO-K1) at 0.25 mg l⁻¹ (4).

Salmonella typhimurium TA98 and TA100 with and without metabolic activation positive (5).

In vitro Chinese hamster ovary cells with and without metabolic activation mutation induction negative (5).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. PAH: maximum admissible concentration 0.2 µg l⁻¹ (6).

Included in Schedule 4 (Release into Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (7).

Other comments

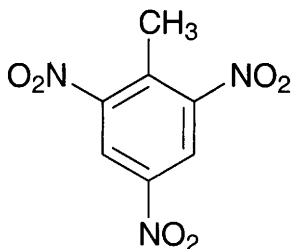
Reviews on human health effects, epidemiology, workplace exposure, experimental toxicology listed (8).

References

1. *Pestic. Toxic. Chem. News* 1980, 8, 4.
2. Seidenberg, J. M. et al *Teratog., Carcinog., Mutagen.* 1986, 6, 361-374.
3. *Report* 8EHQ-0480-0339, United States Environmental Protection Agency, Office of Pesticides and Toxic Substances, 401 M St., SW, Washington, DC, USA.
4. Rodriguez, H. et al *Mutat. Res.* 1990, 240(2), 73-81.

5. Kitchin, R. M. et al *Mutat. Res.* 1988, **206**, 367-377.
6. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
7. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
8. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T331 2,4,6-trinitrotoluene



$C_7H_5N_3O_6$

Mol. Wt. 227.13

CAS Registry No. 118-96-7

Synonyms TNT; α -trinitrotoluol; 2-methyl-1,3,5-trinitrobenzene; Tolit; trinitrotoluene; tritol; trotyl; Trilit

EINECS No. 204-289-6

RTECS No. XU 0175000

Uses Explosive. Intermediate in dyestuffs and photographic chemicals.

Physical properties

M. Pt. 80.1°C **B. Pt.** 240°C **Flash point** explodes **Specific gravity** 1.654 at 20°C with respect to water at 4°C

Volatility v.p. 0.046 mm Hg at 82°C; v.den. 7.85

Solubility Water: 100 mg l⁻¹ at 25°C. Organic solvents: acetone, benzene, ethanol

Occupational exposure

DE-MAK 0.011 ppm (0.1 mg m⁻³)

FR-VME 0.5 mg m⁻³

JP-OEL 0.1 mg m⁻³

SE-LEVL 0.1 mg m⁻³

SE-STEEL 0.2 mg m⁻³

UK-LTEL 0.5 mg m⁻³

US-TWA 0.1 mg m⁻³

UN No. 1356 (wetted with ≥30% water by weight) **Conveyance classification** flammable solid

Supply classification explosive, toxic

Risk phrases Risk of explosion by shock, friction, fire or other sources of ignition – Toxic by inhalation, in contact with skin and if swallowed – Danger of cumulative effects (R2, R23/24/25, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – This material and its container must be disposed of in a safe way – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S35, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow 2.4-2.6 mg l⁻¹ (1,2).

Invertebrate toxicity

EC₅₀ (5 min) *Photobacterium phosphoreum* 19.8 ppm Microtox test (3).

EC₅₀ (48 hr) *Daphnia magna* 11.9 mg l⁻¹ (1).

LOEC *Scenedesmus quadricauda* 1.6 mg l⁻¹ (4).

LOEC *Entosiphon sulcatum* 1.6 mg l⁻¹ (4).

Environmental fate

Degradation studies

Completely degraded by *Pseudomonas fluorescens* B-3468 (5).

In water *Phanerochaete chrysosporium* cultures degraded 50.8 ± 3.2% of [¹⁴C]-labelled compound to ¹⁴CO₂ in 30 days and only 2.8% of the initial TNT could be recovered. In soil, at 30 days, only 6.3 ± 0.6% of the [¹⁴C]-labelled compound was mineralised (6).

Microorganisms isolated from soil and activated carbon from former munition plants were able to degrade >99% TNT in contaminated soil within 14 days (7).

Under strictly anaerobic conditions, an initial concentration of 110 mg l⁻¹ 2,4,6-trinitrotoluene (TNT) was > 99% removed in 6 days by a mixed microbial population in digested sewage culture. Four main metabolites were: 2-hydroxylamino-4,6-dinitrotoluene and its isomer 4-hydroxylamino-2,6-dinitrotoluene; 2-amino-4,6-dinitrotoluene and its isomer 4-amino-2,6-dinitrotoluene. TNT was transformed into 2-amino-4,6-dinitrotoluene via 2-hydroxylamino-4,6-dinitrotoluene and further stepwise deamination and subsequent mineralisation by ring cleavage occurred by mixed specific reductase, which was created by nitro-reducing, sulfate-reducing, methanogenic bacteria (8).

TNT-Contaminated soil from a former ammunition plant was anaerobically fermented in a laboratory slurry reactor by a variety of organisms when electron donors such as glucose were added. During the fermentation of glucose to ethanol, acetate and propionate the nitro groups of 2,4,6-trinitrotoluene were completely reduced, which led to a complete and irreversible binding of the reduced products to the soil. Subsequent aerobic treatment completed the bioremediation process. A technical scale test using a sludge reactor filled with 18 m³ of contaminated soil and 10 m³ of water reduced more than 99% of the contaminants. After anaerobic/aerobic treatment, ecotoxicological tests did not detect any residual toxicity (9,10).

A compost mixture of 50% 2,4,6-trinitrotoluene-contaminated soil, 30% chopped sugar beet, and 20% straw was anaerobically percolated with tap water for 19 days. The water was then drained and the mixture aerated for 58 days. 90% of the trinitrotoluene had been converted into monoaminodinitrotoluenes and diaminomononitrotoluenes (11).

Abiotic removal

In water ~50 and 99% of 260-300 ppm were degraded by UV irradiation at 50°C in the presence of O₂; the major degradation products were 2,3-dinitrophenylamine, 1,3-dinitrobenzene and 1,3,5-trinitrobenzene (12).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 660 and 795 mg kg⁻¹, respectively (13).

LD_{Lo} oral rabbit 500 mg kg⁻¹ (13).

LD_{Lo} subcutaneous cat, rabbit 200 and 500 mg kg⁻¹, respectively (14).

Sub-acute and sub-chronic data

Oral beagle dog (26 wk) 0, 0.5, 2, 8 or 32 mg kg⁻¹ day⁻¹. Major toxic effects included haemolytic anaemia methaemoglobinemia, liver damage and splenomegaly with accompanying histological lesions. Only the highest dose was lethal. Hepatocytic cloudy swelling and hepatocytomegaly were seen in all treated dogs (15).

Teratogenicity and reproductive effects

Oral rat (6-15 day gestation) 1/10 or 1/80 of LD₅₀ dose. Foetal abnormalities were seen mainly in the skeletal system and embryo toxicity appeared as subcutaneous haemorrhage (16).

253 ♀ workers occupationally exposed to TNT showed higher than normal levels of abnormal menstruation, pregnancy disorders, spontaneous abortions and stillbirths (17).

Metabolism and toxicokinetics

Metabolites including 2-amino-4,6-dinitrotoluene, 4-amino-2,6-dinitrotoluene, 2,4-diamino-6-nitrotoluene and 2,6-diamino-4-nitrotoluene were found in the urine of rats and the blood of rabbits fed TNT, in the urine of rats exposed dermally and in the urine of munition workers (18).

Irritancy

Dermal rabbit (24 hr) 500 mg caused mild irritation (19).

Genotoxicity

A CASE study predicted TNT to be mutagenic (20).

Other effects

Other adverse effects (human)

In a survey of 502 exposed workers the rate of eye lens damage was 3.87% and this was related to the concentration of the compound in air and the duration of exposure (21).

Lens opacity was observed in 13.9% of 144 exposed workers and in 6.5% of 77 controls. Of the affected workers, 15% had fine punctiform opacities in the equatorial region 65% had incipient cataracts in the equatorial region and 20% had developed cataract. Lens opacities were found most commonly in workers aged 30-39 yr old following exposure for 5-9 yr, even if the maximum admissible concentration was not exceeded (22).

Workers exposed to TNT from explosives used in open-cut mining showed disorders of the nervous system and peripheral ganglions as well as diseases of the osteomuscular system and the connective tissue. Exposure also aggravated skin diseases, digestive and circulatory system disorders. Temporary disability rates were higher among older workers and those exposed to TNT over a long period of time (23).

Any other adverse effects

Causes liver damage, aplastic anaemia, cyanosis, and mucous membrane or skin irritation (species unspecified) (24).

When administered by gavage to rats, damage to endoplasmic reticulum and mitochondria occurred and inhibition of liver cytochrome P₄₅₀. Simultaneous administration of vitamin E could reduce, but not reverse, the liver damage; cysteine had no effect (25).

Legislation

Included in the UK List of Classified and Authorised Explosives 1994. UK Class and Division 3.2. Competent Authority Reference GB 32348 (26).

Other comments

Explodes at 240°C

References

1. Pearson, J. G. et al *Aquatic Toxicology ASTM STP 667* Marking, L. L. et al (Eds.) 1979, 284-301.
2. Lockhart, W. L. et al *Environ. Physiol. Biochem.* 1975, 5, 361.
3. Kaiser, K. L. E. *Water Pollut. Res. J. Can.* 1991, 26(3), 361-431.
4. Bringmann, G. et al *Water Res.* 1980, 14, 231-241.
5. Naumova, R. P. et al *Mikrobiologiya* 1988, 5(2), 218-222 (Russ.) (*Chem. Abstr.* 109, 20079e).
6. Fernando, T. et al *ACS Symp. Sr.* 1991, 468(Emerging Technol. Hazard Waste Manage. 2), 214-232.
7. Neumeier, W. et al *Forum Staedte-Hyg.* 1989, 40(1), 32-37, (Ger.) (*Chem. Abstr.* 110, 198598g).
8. Kwon, S. H. et al *J. Environ. Sci. Health, Part A: Environ. Sci. Eng. Toxic Hazard. Subst. Control* 1997, A32(9-10), 2669-2682.

9. Lenke, H. et al *Environ. Sci. Technol.* 1998, **32**(13), 1964-1971.
10. Daun, G. et al *Environ. Sci. Technol.* 1998, **32**(13), 1956-1963.
11. Bruns-Nagel, D. et al *Environ. Sci. Technol.* 1998, **32**(11), 1676-1679.
12. Lu, M. et al *Huanjing Kexue* 1987, **8**(2), 15-20 (Ch.) (*Chem. Abstr.* **107**, 12479d).
13. Lewis, R. J. et al *Registry of toxic effects of chemical substances* 1984, National Institute for Occupational Safety and Health No. 83-107-4.
14. *Medical Research Council Special Report Series* 1921, **58**, 32.
15. Levine, B. S. et al *Toxicology* 1990, **63**(2), 233-244.
16. Liu, F. et al *Gongye Weisheng Yu Zhiyebing* 1989, **15**(3), 131-133 (Ch.) (*Chem. Abstr.* **112**, 2452d).
17. Yang, S. *Gongye Weisheng Yu Zhiyebing* 1994, **20**(1) (Chinese) (*Chem. Abstr.* **122**(12) 141229).
18. Yinon, J. et al *J. Energ. Mater.* 1986, **4**(1-4), 305-313.
19. *National Technical Information Service* AD-B011-150.
20. Klopman, G. et al *Mutat. Res.* 1990, **228**(1), 1-50.
21. Zhang, H. *Zhonghua Laodong Weisheng Zhiyebing Zazhi* 1988, **6**(3), 133-136 (Ch.) (*Chem. Abstr.* **112**, 144862m).
22. Perunicic, B. et al *Prac. Lek.* 1990, **42**(6), 252-254 (Czech.) (*Chem. Abstr.* **115**, 98343e).
23. Vysochin, V. I. *Gig. Tr. Prof. Zabol.* 1987, **12**, 40-44 (Russ.) (*Chem. Abstr.* **108**, 81182j).
24. Clayton, G. D. et al (Eds.) *Patty's Industrial Hygiene and Toxicology* 3rd rev. ed., 1981, **2A**, John Wiley & Sons, New York, NY, USA.
25. Wang, R. et al *Weisheng Dulixue Zazhi* 1988, **2**(1), 41-45 (Ch.) (*Chem. Abstr.* **112**, 51088u).
26. *UK Explosives Acts, 1875 and 1923. The Classification and Labelling of Explosives Regulations 1983 (CLER). List of Classified and Authorised Explosives 1994 (LOCAE) 1994*, HSE, UK

T332 trioctyl phosphate



$\text{C}_{24}\text{H}_{51}\text{O}_4\text{P}$

Mol. Wt. 434.64

CAS Registry No. 1806-54-8

Synonyms phosphoric acid, trioctyl ester; tri-*n*-octyl phosphate

EINECS No. 217-305-1

Physical properties

M. Pt. 52°C B. Pt. 228-233°C at 6 mmHg Specific gravity 0.92 at 20°C

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535 and TA1537 with and without metabolic activation negative (1).

Legislation

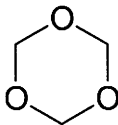
Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phosphorus: guide level 400 µg l⁻¹, maximum admissible concentration 5000 µg l⁻¹ (2).

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (3).

References

1. Zeiger, E. et al *Environ. Mutagen* 1987, **9**(Suppl. 9), 1-109.
2. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
3. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T333 1,3,5-trioxane



$C_3H_6O_3$

Mol. Wt. 90.08

CAS Registry No. 110-88-3

Synonyms s-trioxane; Triformol; trioxymethylene

EINECS No. 203-812-5

RTECS No. YK 0350000

Physical properties

M. Pt. 64°C B. Pt. 114.5°C at 759 mmHg Flash point 45°C (open cup) Specific gravity 1.17

Volatility v.p. 13 mmHg at 25°C; v.den. 3.1

Solubility Water: 211 g l⁻¹ at 25°C. Organic solvents: acetone, diethyl ether, ethanol, light petroleum

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed (R22)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with skin and eyes (S2, S24/25)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) salmon 60 mg l⁻¹ (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 800 mg kg⁻¹ (2).

LD_{Lo} dermal rabbit 10,000 mg kg⁻¹ (3).

Sub-acute and sub-chronic data

Intragastric (duration unspecified) rat 10, 20, 80 mg kg⁻¹ caused no observable toxic effects (4,5).

Metabolism and toxicokinetics

¹⁴C-labelled trioxane (400 mg kg⁻¹) was administered to rats (route unspecified). 77% of the radio-label was exhaled as CO₂, 8% as unchanged trioxane and 3% was excreted in urine as unchanged trioxane (6).

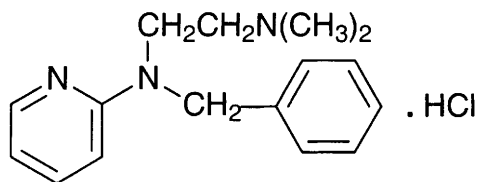
Irritancy

Dermal rabbit 500 mg (24 hr) caused severe irritation and 100 mg instilled into rabbit eye (72 hr) caused severe irritation (3).

References

1. Sprague, J. B. et al *Environ. Poll.* 1979, **19**, 269.
2. Frear, E. H. (Ed.) *Pesticide Index* 1969, College Science Publications, State College, PA, USA.
3. *Data Sheet* BIOFAX Industrial Bio-Test Laboratories, Inc., 1810 Frontage Road, Northbrook, IL, USA.
4. Czajkowska, T. et al *Med. Pr.* 1987, **38**(4), 244-249.
5. Czajkowska, E. et al *Med. Pr.* 1987, **38**(3), 184-190.
6. Ligocka, D. et al *Arch. Toxicol.* 1998, **72**(5), 303-308

T334 tripelennamine hydrochloride



$C_{16}H_{22}ClN_3$

Mol. Wt. 291.82

CAS Registry No. 154-69-8

Synonyms *N,N*-dimethyl-*N'*-(phenylmethyl)-*N'*-2-pyridinyl-1,2-ethanediamine, monohydrochloride; Dehistin; Piristin; Stanzamine; Pyrinamine; Resistamine

EINECS No. 205-833-5

RTECS No. US 3150000

Uses Antihistamine.

Physical properties

M. Pt. 192-193°C

Solubility Water: 1.29 kg l⁻¹. Organic solvents: diethyl ether, chloroform, ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, guinea pig, rat, 97, 155, 515 mg kg⁻¹, respectively (1,2,3).

LD₅₀ subcutaneous guinea pig, rabbit, mouse, rat 30, 33, 41, 225 mg kg⁻¹, respectively (2,3).

LD₅₀ intravenous rabbit, mouse, rat, hamster 9, 9, 12, 13 mg kg⁻¹, respectively (3,4,5).

LD₅₀ intraperitoneal mouse 47 mg kg⁻¹ (6).

Other effects

Other adverse effects (human)

Severe toxic reaction, including agitation and hallucinations, occurred in an 8-yr-old child who was sprayed over the body (7).

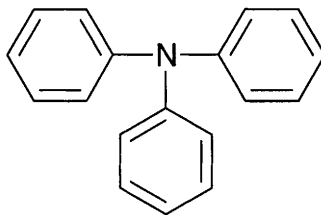
Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (8).

References

1. *J. Pharmacol. Exp. Ther.* 1950, **9**, 488.
2. *J. Pharmacol. Exp. Ther.* 1955, **113**, 572.
3. *J. Lab. Clin. Med.* 1946, **31**, 749.
4. *J. Pharmacol. Exp. Ther.* 1948, **92**, 249.
5. *J. Pharmacol. Exp. Ther.* 1949, **97**, 371.
6. *Clin. Toxicol.* 1980, **16**, 17.
7. Schipior, P. G. *J. Pediatr.* 1967, **71**, 589-591.
8. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

T335 triphenylamine



C₁₈H₁₅N

Mol. Wt. 245.32

CAS Registry No. 603-34-9

Synonyms *N,N*-diphenylbenzenamine; *N,N*-diphenylaniline

EINECS No. 210-035-5

RTECS No. YK 2680000

Physical properties

M. Pt. 125-127°C B. Pt. 347-348°C Flash point 180°C (open cup) Specific gravity 0.774 at 0°C with respect to water at 0°C Partition coefficient log P_{ow} 5.74

Occupational exposure

FR-VME 5 mg m⁻³

US-TWA 5 mg m⁻³

Ecotoxicity

Invertebrate toxicity

EC₅₀ (5 min) *Photobacterium phosphoreum* 1.66 ppm Microtox test (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 1600, 3200 mg kg⁻¹, respectively (2).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537, with and without metabolic activation negative (3).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phenols: maximum admissible concentration 0.5 µg l⁻¹ (4).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (5).

Other comments

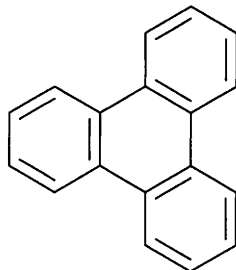
Reviews on human health effects, experimental toxicity and workplace experience listed (6).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, 26(3), 361-431.
2. *Documentation of the threshold limit values and biological exposure indices* 5th ed., 1986, 612, American Conference of Governmental Industrial Hygienists, Cincinnati, OH, USA.
3. Zeiger, E. et al *Environ. Mol. Mutagen.* 1987, 9(Suppl. 9), 1-109.
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.

5. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
6. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T336 triphenylene



C₁₈H₁₂

Mol. Wt. 228.29

CAS Registry No. 217-59-4

Synonyms benzo[1]phenanthrene; 9,10-benzophenanthrene; isochrysene

EINECS No. 205-922-9

RTECS No. YK 2925000

Occurrence In fossil fuels; in mainstream cigarette smoke, petrol engine exhaust and exhaust tar (1-3).

Physical properties

M. Pt. 197-200°C **B. Pt.** 438°C **Specific gravity** 1.302 **Partition coefficient** log P_{ow} 5.49

Solubility Water: 38 µg l⁻¹. Organic solvents: acetic acid, benzene, chloroform, ethanol

Ecotoxicity

Bioaccumulation

Mean concentration in soft parts of *Mytilus edulis* 85 ng g⁻¹ dry weight. Mean concentration in gallbladder of *Somateria mollissima* 14 ng g⁻¹ dry weight (4).

Mammalian & avian toxicity

Carcinogenicity and chronic effects

Dermal (548 day) 10 mice painted twice weekly with 0.3% solution in benzene. No skin lesion was observed (5).

Dermal (82 wk) 20 C3 H mice, 60 µl of a 0.5% solution. No skin tumours were observed (6).

Genotoxicity

Salmonella typhimurium his⁻/+ with metabolic activation positive (7,8).

Salmonella typhimurium 8AGS/R with metabolic activation positive (9).

Salmonella typhimurium TA100 with metabolic activation positive (10).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. PAH: maximum admissible concentration 0.2 µg l⁻¹ (11).

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (12).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (13).

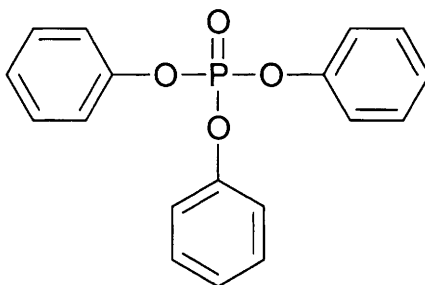
Other comments

Reviews on human health effects and experimental toxicity listed (14).

References

1. Snook, M. E. et al *Beitr. Tabakforsch. Int.* 1977, **9**, 79-101.
2. Grimmer, G. et al *Zbl. Bakt. Hyg., 1 Abt., Orig.* 1977, B164, 218-234.
3. Hoffman, D. et al *Cancer* 1962, **15**, 93-102.
4. Broman, D. et al *Environ. Toxicol. Chem.* 1990, **9**, 429-442.
5. Barry, G. et al *Part III. Proc. R. Soc. London Ser. B* 1935, **117**, 318-351.
6. Horton, A. W. et al *J. Natl. Cancer Inst.* 1974, **53**, 1017-1020.
7. Mossanda, K. et al *Food Cosmet. Toxicol.* 1979, **17**, 141-143.
8. Wood, A. W. et al *Cancer Res.* 1980, **40**, 1985-1989.
9. Kaden D. A. et al *Cancer Res.* 1979, **39**, 4152-4159.
10. Pahlman, R. et al *Carcinogenesis* 1987, **8**(6), 773-778.
11. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
12. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
13. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; *6th Amendment EEC Directive* 79/831/EEC; *7th Amendment EEC Directive* 91/32/EEC 1991, HMSO, London, UK.
14. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T337 triphenyl phosphate



C₁₈H₁₅O₄P

Mol. Wt. 326.29

CAS Registry No. 115-86-6

Synonyms Celluflux TPP; Disflamoll TP; Phosflex TPP; TPP; triphenoxyphosphine oxide

EINECS No. 204-112-2

RTECS No. TC 8400000

Uses Catalyst. Plasticiser. Fire-proofing agent. Lubricating oil additive. Antioxidant. Insecticide.

Physical properties

M. Pt. 50-52°C **B. Pt.** 260°C **Flash point** 223°C **Specific gravity** 1.2055 at 50°C with respect to water at 4°C

Volatility v.p. 1 mmHg at 193.5°C; v.den. 11.3

Solubility Water: 0.002% at 54°C. Organic solvents: acetone, benzene, carbon tetrachloride, chloroform, diethyl ether, ethanol

Occupational exposure

FR-VME 3 mg m⁻³

UK-LTEL 3 mg m⁻³

US-TWA 3 mg m⁻³

UK-STEL 6 mg m⁻³

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow, rainbow trout 300-870 mg l⁻¹ static bioassay (1,2).

LC₅₀ (96 hr) bluegill sunfish, inland silverside 95 and 290 mg l⁻¹, respectively, static bioassay (3).

Environmental fate

Degradation studies

Biodegradation in sediment t_{1/2} 2-8 days at 25°C, 11.9 days at 2°C (4).

Degraded by bacteria in the river water of Osaka City in < 5 days (5).

Abiotic removal

Hydrolysis t_{1/2} 1.3 day at pH 9.5; 7.5 day at pH 8.2 (6).

Degraded by combined treatment with UV irradiation and hydrogen peroxide in water (7).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse, chicken 1.3-10.8 g kg⁻¹ (8-10).

LD₅₀ dermal rabbit >7900 mg kg⁻¹ (10).

LD₅₀ intraperitoneal mouse 1300 mg kg⁻¹ (11).

LD₅₀ subcutaneous cat 100 mg kg⁻¹ (12).

Sub-acute and sub-chronic data

Oral rat 0, 0.25, 0.5, 0.75 or 1.0% diet for 120 days. No significant effects were observed in immunotoxicity, as assessed by humoral response to a T-lymphocyte-dependent antigen and sheep red blood cells (13).

Oral rat 0, 0.25, 0.5, 0.75 or 1% diet for 4 months. At levels >0.25% diet there were treatment-related decreases in weight gain. Neuromotor functional tests showed no adverse effects (14).

Metabolism and toxicokinetics

Metabolised by rat liver microsomes *in vitro* to diphenyl phosphate in the presence and absence of NADPH. The reaction was linked to cytochrome P₄₅₀ (15).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (16).

Other effects

Any other adverse effects

Inhibited cholinesterase (8).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phosphorus: guide level 400 µg l⁻¹; maximum admissible concentration 5000 µg l⁻¹ (as P₂O₅) (17).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (17).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (18).

Other comments

Metabolism by carboxyesterases and human monocytes studied (19).

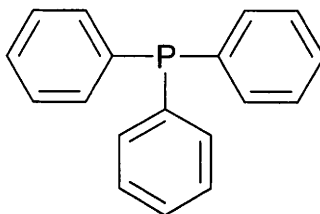
Physical properties, metabolism and toxicity reviewed (20).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (21).

References

1. Litthichaikasen, S. *Diss. Abstr.* 1978, **39**, 7813246.
2. Gaizer, D. L. et al *Acute Toxicities of Organic Chemicals to Fathead Minnows* 1986, **3**, 311, University of Wisconsin, Lake Superior, USA.
3. Dawson, G. W et al *J. Haz. Mat.* 1975/77, **1**, 303-318.
4. Muir, D. C. G. *Toxicol. Environ. Chem.* 1989, **18**(4), 269-286.
5. Kawai, S. et al *Ann. Rep. Osaka City Inst. Public Health Environ. Sci.* 1985, **48**, 175-183 (Japan.)(*Chem. Abstr.* **107**, 28119x).
6. Howard, P. H. et al *Bull. Environ. Contam. Toxicol.* 1979, **22**, 337-344.
7. Thiermann, W. et al *DVGW – Schriftnr. Wasser* 1988, **107**, 129-146 (Ger.)(*Chem. Abstr.* **110**, 101421h).
8. *Documentation for Threshold Limit Values for Substances in Workroom Air* 4th ed., 1980, 420, American Conference of Governmental Industrial Hygienists, Cincinnati, OH, USA.
9. *Arzneim.-Forsch.* 1957, **7**, 585.
10. Johannsen, F. R. et al *Toxicol. Appl. Pharmacol.* 1977, **41**, 291-304.
11. *Agric. Biol. Chem.* 1967, **31**, 1288.
12. *Patty's Industrial Hygiene and Toxicology* 2nd ed., 1963, 916, Wiley Interscience, New York, NY, USA.
13. Hinton, D. M. et al *Toxicol. Ind. Health* 1987, **3**(1), 71-89.
14. Sobotka, T. J. et al *Neurobehav. Toxicol. Teratol.* 1986, **8**, 7-10.
15. Sasaki, K. et al *Bull. Environ. Contam. Toxicol.* 1984, **33**, 281-288.
16. Zeiger, E. et al *Environ. Mol. Mutagen.* 1987, **9** (Suppl.9), 1-109.
17. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
18. *S. I. No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
19. Paxman, D. G. *Diss. Abstr. Int. B* 1989, **50**(1), 106-107.
20. Snyder, R. *Ethel Browning's Toxicity and Metabolism of Industrial Solvents* 2nd ed., 1990, 2, 487-493, Elsevier, New York, NY, USA.
21. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T338 triphenylphosphine



C₁₈H₁₅P

Mol. Wt. 262.29

CAS Registry No. 603-35-0

Synonyms triphenylphosphane; triphenyl phosphide; triphenylphosphorus

EINECS No. 210-036-0

RTECS No. SZ 3500000

Uses In organic synthesis. Polymerisation initiator.

Physical properties

M. Pt. 79°C B. Pt. >360°C Flash point 180°C (open cup) Specific gravity 1.194 Partition coefficient log P_{ow} 4.5 (1) Volatility v.den. 9.0
Solubility Organic solvents: benzene, diethyl ether, ethanol

Ecotoxicity

Invertebrate toxicity

EC₅₀ (5 min) *Photobacterium phosphoreum* 1.54 ppm Microtox test (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 800 mg kg⁻¹ (3).

LC₅₀ (4 hr) inhalation rat 1135 ppm (4).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535 and TA1537 with and without metabolic activation negative (5).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phenols: maximum admissible concentration 0.5 µg l⁻¹ (6).

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (7).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (8).

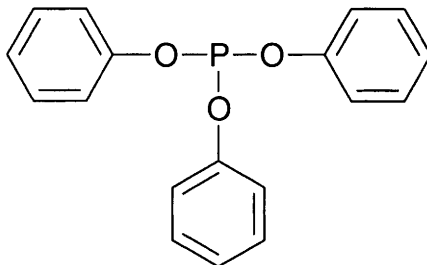
Other comments

Reviews on human health effects, experimental toxicity and workplace experience listed (9).

References

1. Kaiser, K. L. E. et al *QSAR Environ. Toxicol. Proc. Int. Workshop* 1987, 2, 153-168.
2. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, 26(3), 361-431.
3. Patty, F. A. (Ed.) *Industrial Hygiene and Toxicology* 2nd ed. 1963, Interscience Publishers, New York, NY, USA.
4. *Annual Meeting of American Industrial Hygiene Association* 1969, AIHA, 475 Wolf Ledges Parkway, Adron, OH, USA.
5. Zeiger, E. et al *Environ. Mol. Mutagen.* 1987, 9(Suppl. 9), 1-109.
6. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
7. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
8. *1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; *6th Amendment EEC Directive* 79/831/EEC; *7th Amendment EEC Directive* 91/32/EEC 1991, HMSO, London, UK.
9. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T339 triphenyl phosphite



$C_{18}H_{15}O_3P$

Mol. Wt. 310.29

CAS Registry No. 101-02-0

Synonyms phosphorous acid, triphenyl ester; phenyl phosphite; Advance TJP360; Mellite 310; TPP

EINECS No. 202-908-4

RTECS No. TH 1575000

Physical properties

M. Pt. 22-25°C B. Pt. 155-160°C at 0.1 mmHg Flash point 218°C (open cup) Specific gravity 1.184 at 25°C with respect to water at 25°C

Occupational exposure

Supply classification irritant

Risk phrases Irritating to eyes and skin (R36/38)

Safety phrases Keep out of reach of children (if sold to general public) – After contact with skin, wash immediately with plenty of water (S2, S28)

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 1333, 1600 mg kg⁻¹, respectively (1,2).

LD₅₀ intraperitoneal mouse 1167 mg kg⁻¹ (3).

LD_{Lo} subcutaneous cat, rat 300, 2000 mg kg⁻¹, respectively (4).

Metabolism and toxicokinetics

Subcutaneous hens, 1000 mg kg⁻¹ triphenyl phosphite was converted into diphenyl phosphonic acid (5).

Irritancy

Dermal human (48 hr) 125 mg caused severe irritation (3).

Dermal rabbit 500 mg (24 hr) caused moderate irritation and 500 mg instilled into rabbit eye (24 hr) caused mild irritation (6).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (7).

Other effects

Any other adverse effects

Neuropathy was reported in rats and hens following subcutaneous administration (8,9).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phenols: maximum admissible concentration $0.5 \mu\text{g l}^{-1}$; Phosphorus: guide level $400 \mu\text{g l}^{-1}$; maximum admissible concentration $5000 \mu\text{g l}^{-1}$ (10). Included in Schedule 5 (Release into Water: Prescribed Substances) Statutory Instrument No. 472, 1991 (11).

Other comments

Neurotoxicity and skin irritancy has been reported (12).

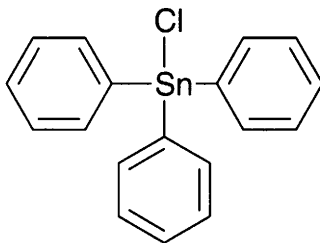
Reviews on human health effects, experimental toxicity, environmental effects, ecotoxicity, exposure levels and hazard assessment listed (13).

Hazard, neurotoxicity and human dermal irritation reviewed (14).

References

1. *Gig. Tr. Prof. Zabol.* 1973, **17**(10), 38.
2. Patty, F. A. (Ed.) *Industrial Hygiene and Toxicology* 2nd rev. ed., 1963, **2**, 1918, Interscience Publishers, New York, NY, USA.
3. *AMA, Arch. Ind. Hyg. Occup. Med.* 1952, **5**, 31.
4. *J. Pharmacol. Exp. Ther.* 1933, **49**, 78.
5. Carrington, C. D. et al *Drug Metab. Dispos.* 1988, **16**(1), 104-109.
6. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
7. Zeiger, E. et al *Environ. Mol. Mutagen.* 1987, **9**(Suppl. 9), 1-109.
8. Veronesi, B. et al *Neuropathol. Appl. Neurobiol.* 1987, **13**(3), 193-208.
9. Carrington, C. D. et al *Neurotoxicology* 1988, **9**(2), 223-233.
10. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
11. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
12. Faust, R. A. et al *NTIS Report* 1986, ORNL-6347; Order No. DE87005378.
13. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
14. Faust, R.A. et al *Energy Res. Abstr.* 1987, **12**(12), Abstr. No. 25981

T340 triphenyltin chloride



$\text{C}_{18}\text{H}_{15}\text{ClSn}$

Mol. Wt. 385.48

CAS Registry No. 639-58-7

Synonyms chlorotriphenyl stannane; brestanol; fentin chloride; triphenylchlorostannane; GC 8993; LS4442

EINECS No. 211-358-4

RTECS No. WH 6860000

Physical properties

M. Pt. 108°C (decomp.) (95% purity) B. Pt. 240°C at 13.55 mmHg

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Sn) (total dust)

SE-LEVL 0.1 mg m⁻³ (as Sn)

SE-STEL 0.2 mg m⁻³ (as Sn)

UK-LTEL 0.1 mg m⁻³ (as Sn)

UK-STEL 0.2 mg m⁻³ (as Sn)

US-TWA 0.1 mg m⁻³ (as Sn)

US-STEL 0.2 mg m⁻³ (as Sn)

UN No. 2788 (liquid)

UN No. 3146 (solid) HAZCHEM Code 2X (solid) Conveyance classification toxic substance

Supply classification toxic

Risk phrases Toxic by inhalation, in contact with skin and if swallowed (R23/24/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Take off immediately all contaminated clothing – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S26, S27, S28, S45)

Ecotoxicity

Invertebrate toxicity

LC₅₀ (duration unspecified) *Selenastrum quadricauda* 0.04 mg l⁻¹ (1).

EC₅₀ (72 hr) *Skeletonema costatum* 0.0092 mg l⁻¹ (2).

EC₅₀ (30 min) *Photobacterium phosphoreum* 0.0157 ppm Microtox test (3).

Environmental fate

Abiotic removal

Ultraviolet irradiation of a solution yielded a mixture of triphenyl-, diphenyl-, and phenyltin in addition to inorganic compounds, within 6 hr (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 18, 135 mg kg⁻¹, respectively (5).

LD₅₀ intravenous mouse 18 mg kg⁻¹ (6).

Other effects

Any other adverse effects

Oral guinea pig (dose and duration unspecified) lethargy and histological changes in the liver and spleen were observed. A decreased immunological response with a reduction in the number of leukocytes and of plasma cells in the lymph nodes of guinea pigs has been observed (7).

Legislation

Included in Schedules 5 and 6 (Release into the Water/Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (8).

Other comments

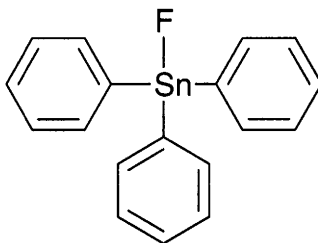
Interactions between dissolved humic material (DHM) and triphenyl tin chloride increase the EC₅₀ values observed for *Daphnia magna* to an extent dependent on the source and concentration of the DHM (9).

Organotins (unspecified) enhanced the induction of chromatid aberrations by clastogenic pollutants in chlorinated tap water, indicating a potential increased risk to health (10).

References

1. Wong, P. T. S. et al *Can J. Fish. Aquat. Sci.* 1982, **39**, 483.
2. Walsh, G. E. et al *Chemosphere* 1985, **14**, 383-389.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. Akahi, H. et al *J. Food Hyg.* 1972, **13**, 85-88.
5. *Farm Chemicals Handbook* 1983, **C245**, Meister Publishing Co., Willoughby, OH, USA.
6. *Report NX 01649*, US Army Armament Research and Development Command, Chemical Systems Laboratory, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD, USA.
7. *Environmental Health Criteria 15. Tin and Organotin Compounds* 1980, WHO, Geneva, Switzerland.
8. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
9. Bao, M.L. et al *Bull. Environ. Contam. Toxicol.* 1997, **59**(4), 671-676.
10. Sasaki, Y. F. *Mutat. Res.* 1993, **300**(1), 5-14

T341 triphenyltin fluoride



$C_{18}H_{15}FSn$

Mol. Wt. 369.03

CAS Registry No. 379-52-2

Synonyms fluorotriphenylstannane; BioMeT 204

EINECS No. 206-833-8

RTECS No. WH 8275500

Physical properties

M. Pt. $>281^{\circ}C$

Occupational exposure

DE-MAK 0.1 mg m^{-3} (as Sn) (total dust)

SE-LEVL 0.1 mg m^{-3} (as Sn)

SE-STEEL 0.2 mg m^{-3} (as Sn)

UK-LTEL 0.1 mg m^{-3} (as Sn)

UK-STEEL 0.2 mg m^{-3} (as Sn)

US-TWA 0.1 mg m^{-3} (as Sn)

US-STEEL 0.1 mg m^{-3} (as Sn)

UN No. 2788 (liquid)

UN No. 3146 (solid) HAZCHEM Code 2X (solid) Conveyance classification toxic substance

Supply classification toxic

Risk phrases Toxic by inhalation, in contact with skin and if swallowed (R23/24/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Take off immediately all contaminated clothing – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S26, S27, S28, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bleak 0.4 mg l^{-1} (1).

Invertebrate toxicity

LC₅₀ (96 hr) *Nitocra spinipes* 0.008 mg l⁻¹ (1).

Other effects**Any other adverse effects**

The antiaggregating (IC₅₀) concentration was 6×10^{-6} M against collagen in rabbits. The collagen and thrombin-induced formation of malondialdehyde was inhibited. Inhibition of collagen-induced arachidonic acid release from platelet phospholipids was due to its action on phospholipase A₂ activity (2,3).

Oral rabbit 100 mg kg⁻¹ caused hypertriglyceridaemia. The compound interfered with insulin release from rabbit β-cells and/or decreased the sensitivity of islets to release insulin in response to increasing levels of blood glucose (4,5).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (6).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (7).

Other comments

Organotins (unspecified) enhanced the induction of chromatid aberrations by clastogenic pollutants in chlorinated tap water, indicating a potential increased risk to health (8).

References

1. Linden, E. et al *Chemosphere* 1979, **11/12**, 843-851.
2. Manabe, S. et al *Sangyo Igaku* 1983, **25**(1), 15-22.
3. Manabe, S. et al *Biochem. Pharmacol.* 1983, **32**(10), 1627-1634.
4. Manabe, S. et al *J. Jpn. Diabetic Soc.* 1981, **24**(6), 669-677.
5. Manabe, S. et al *Diabetes* 1981, **30**(12), 1013-1021.
6. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
7. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
8. Sasaki, Y. F. et al *Mutat. Res.* 1993, **300**(1), 5-14

T342 tripropylamine

C₉H₂₁N

Mol. Wt. 143.27

CAS Registry No. 102-69-2

Synonyms *N,N*-dipropyl-1-propylamine

EINECS No. 203-047-7

RTECS No. TX 1575000

Physical properties

M. Pt. -93.5°C B. Pt. 155-158°C Flash point 36°C (open cup) Specific gravity 0.75 Partition coefficient log P_{ow} 2.79 Volatility v.den. 4.9

Occupational exposure

UN No. 2260 HAZCHEM Code 3W Conveyance classification flammable liquid, corrosive

Ecotoxicity

Toxicity to other species

Minimum toxic concentration for tadpoles 36 mg l⁻¹ (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 72 mg kg⁻¹ (2).

LC₅₀ (2 hr) inhalation mouse 3800 mg m⁻³ (3).

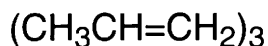
LC_{Lo} (4 hr) inhalation rat 250 ppm (2).

LD₅₀ dermal rabbit 429 mg kg⁻¹ (2).

References

1. Colosi-Esca, D. et al *Rev. Chim. (Bucharest)* 1987, **38**(10), 933-937.
2. *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 470.
3. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR

T343 tripropylene



C₉H₁₈

Mol. Wt. 126.24

CAS Registry No. 13987-01-4

Synonyms 1-propene trimer; tri-*n*-propylene

Physical properties

M. Pt. -93.5°C B. Pt. 156°C Specific gravity 0.757 at 20°C with respect to water at 4°C

Partition coefficient log P_{ow} 2.79 (1) Volatility v.den. 4.9

Occupational exposure

UN No. 2057 HAZCHEM Code 3ME Conveyance classification flammable liquid

Ecotoxicity

Fish toxicity

LC_{Lo} (24 hr) creek chub 30 mg l⁻¹ (2).

LC₁₀₀ (24 hr) creek chub 70 mg l⁻¹ (2).

Environmental fate

Degradation studies

Can be degraded by *Aerobacter* sp. at 30°C (3).

References

1. Vershueren, K. *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, Van Nostrand Reinhold, New York, NY, USA.
2. Gillette, L. A. *Sewage Ind. Wastes* 1952, **24**(11), 1397-1401.
3. Worne, H.. E. *Tijdschrift van hert BECEWA*, Liege, Belgium

T344 tripropyltin oxide



$\text{C}_{18}\text{H}_{42}\text{OSn}_2$

Mol. Wt. 511.95

CAS Registry No. 1067-29-4

Synonyms bis(tripropyltin) oxide; hexapropyl-distannoxane; tripropyltin oxide

EINECS No. 213-927-2

RTECS No. JN 8800000

Uses Antifouling agent used in marine paints.

Occupational exposure

DE-MAK 0.1 mg m⁻³ (as Sn) (total dust)

FR-VME 0.1 ppm m⁻³ (as Sn)

SE-LEVL 0.1 mg m⁻³ (as Sn)

SE-STEL 0.2 mg m⁻³ (as Sn)

UK-LTEL 0.1 mg m⁻³ (as Sn)

UK-STEL 0.2 mg m⁻³ (as Sn)

US-TWA 0.1 mg m⁻³ (as Sn)

US-STEL 0.2 mg m⁻³ (as Sn)

UN No. 2788 (liquid)

UN No. 3146 (solid) **HAZCHEM Code** 2X (solid) **Conveyance classification** toxic substance

Supply classification toxic

Risk phrases Toxic by inhalation, in contact with skin and if swallowed (R23/24/25)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Take off immediately all contaminated clothing – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S26, S27, S28, S45)

Ecotoxicity

Invertebrate toxicity

Mud crabs exposed to tripropyltin oxide exhibit acute and sub-lethal effects on development rate and growth of larvae (1).

The relationships between this toxicity and physical properties has been assessed (2).

Environmental fate

Degradation studies

Organotins can be degraded by light, but light may also stimulate photosynthetic organisms which can carry out degradation (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral blackbird 40 mg kg⁻¹ (4).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (5).

Included in Control of Pollution (Anti-fouling Paints and Treatments) Regulations 1987 (6).

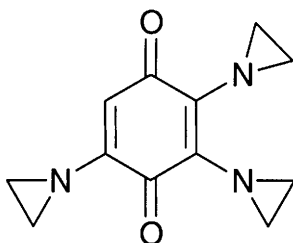
Other comments

Toxicity reviewed (7,8).

References

1. Laughlin, R. B. et al *Environ. Toxicol. Chem.* 1985, **4**(3), 343-351.
2. Laughlin, R. B. et al *QSAR Environ. Toxicol. Pro. Int. Workshop* 2nd 1986, 189-206.
3. *The Biological Alkylation of Heavy Elements* 1987, (Ed.) P. J. Craig, et al, The Royal Society of Chemistry, London, UK.
4. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
5. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
6. S. I. 1987, No. 783 *Control of Pollution (Anti-fouling Paints and Treatments) Regulations* 1987, HMSO, London, UK.
7. Thomson, J. A. J. et al *Organotin Compounds in the Aquatic Environment* 1985, NRCC, Assoc. Comm. Scientific Criteria Qualit. Publ. No. NRCC 2294 Nat. Res. Coun., Canada.
8. Thayer, J. S. et al *Adv. Organomet. Chem.* 1982, **20**, 313

T345 2,3,5-tris(1-aziridiny)-p-benzoquinone



$C_{12}H_{13}N_3O_2$

Mol. Wt. 231.25

CAS Registry No. 68-76-8

Synonyms triaziquone; 2,3,5-tris(1-aziridiny)-2,5-cyclohexadiene-1,4-dione; Trenimon; Prenimon

EINECS No. 200-692-6

RTECS No. DK 7175000

Uses Antineoplastic agent.

Physical properties

M. Pt. 162-163°C

Solubility Organic solvents: acetone, benzene, methanol

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat 161 mg kg⁻¹ (1).

LD₅₀ intravenous rat 470 µg kg⁻¹ (2).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (3).

♂ Rats injected with 30 µg kg⁻¹ wk⁻¹ for 1 yr developed a significant number of malignant tumours after ≤19 months. The majority were sarcomas of the abdominal cavity (2).

♂ Rats injected once wkly for ~25 wk with 30 µg kg⁻¹, and then with the same dose intraperitoneally for 33 wk, developed a significant number of malignant tumours (4).

Tested positive in the initiator tRNA acceptance assay for carcinogens (5).

Teratogenicity and reproductive effects

In vitro effects on growth and differentiation of mouse embryos in culture have been demonstrated (6).

Genotoxicity

Alkylating agent capable of alkylating DNA *in vitro* (7).

Saccharomyces cerevisiae gene conversion without metabolic activation positive (8).

Drosophila melanogaster sex chromosome loss and formation of sex-linked recessive lethals positive (9,10).

In vitro chromosome aberrations in human lymphocytes without metabolic activation positive (11).

Drosophila melanogaster DNA lesions positive (12).

Other effects

Any other adverse effects

Leucopenia has been reported in patients receiving the compound therapeutically.

At autopsy patients were reported to have neoplastic reticulosis in bone marrow, spleen and lymph nodes (13).

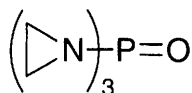
Other comments

Toxicology and mutagenicity of the compound reviewed (14,15).

References

1. *Arzneim.-Forsch.* 1966, **16**, 1533.
2. Schmaehl, D. et al *Arzneim.-Forsch.* 1970, **20**, 1461-1467.
3. *IARC Monograph* 1987, **Suppl.** 7, 367.
4. Schmahl, D. *Dtsch. Med. Wochenschr.* 1967, **92**, 1150-1152.
5. Hradec, J. *Carcinogenesis (London)* 1989, **10** (8), 1413-1417.
6. Van Maele-Fabry, G. et al *Teratology* 1987, **36** (1), 95-106.
7. Klamerth, O. L. et al *Eur. J. Biochem.* 1971, **21**, 199-203.
8. Zimmermann, F. K. *Mutat. Res.* 1971, **11**, 327-337.
9. Mollet, P. *Mutat. Res.* 1973, **21**, 135-148.
10. Vogel, E. W. *Mutat. Res.* 1973, **20**, (1), 339-352.
11. Hager, et al *Hum. Genet.* 1982, **61**, 342-356.
12. Vogel, E. W. *Mutat. Res.* 1989, **211**, (1), 153-170.
13. Terbruggen, A. *Dtsch. Ges. Path.* 1965, **49**, 241-245.
14. *IARC Monograph* 1975, **9**, 67.
15. *IARC Monograph* 1987, **Suppl.** 6, 545

T346 tris(1-aziridinyl)phosphine oxide



$C_6H_{12}N_3OP$

Mol. Wt. 173.15

CAS Registry No. 545-55-1

Synonyms 1,1',1''-phosphinylidynetrisaziridine; tris(1-aziridinyl)phosphine oxide; phosphoric acid triethylene imide; Aphoxide; TEPA; APO

EINECS No. 208-892-5

RTECS No. SZ 1750000

Uses Used in dyeing, creaseproofing and flameproofing textiles. Stabiliser for polymers. In photographic emulsion hardening. Antineoplastic agent. Insect sterilant.

Physical properties

M. Pt. 41°C B. Pt. 90-91°C at 23°C

Solubility Organic solvents: acetone, diethyl ether, ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 37 mg kg⁻¹ (1).

LD_{Lo} intraperitoneal mouse 156 µg kg⁻¹ (2).

LD₅₀ intravenous mouse 178 mg kg⁻¹ (3).

Carcinogenicity and chronic effects

No adequate data for carcinogenicity to humans, inadequate evidence for carcinogenicity to animals, IARC classification group 3 (4).

Metabolism and toxicokinetics

Excreted in urine as a thiophosphamide metabolite (5).

Intraperitoneal rat and mouse (dose unspecified), radioactivity was not localised selectively in any of the tissues examined. During first 24 hr after treatment, 60-75% of dose excreted in urine, 2-5% in faeces in mouse, with 80% of radioactivity identified as inorganic phosphate. In rat, 80% of radioactivity in blood, associated with haemoglobin. During first 24 hr, 89-90% of radioactivity excreted in urine; 50-70% of urinary radioactivity was present as unchanged tris(1-aziridinyl)phosphine oxide (6).

The sperm-rich fraction of boar semen was treated *in vitro* for 10 min with an equal volume of 1% solution. On average, 0.8% was taken up in the spermatozoa, 69% was associated with the heads and 31% with the tails and acrosomes (7).

Genotoxicity

Drosophila melanogaster wing spot test positive (8).

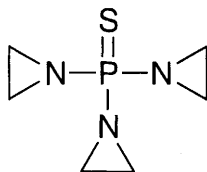
Other comments

Human health effects and experimental toxicology reviewed (6,9).

References

1. Bull. World Health Organisation 1964, **31**, 737.
2. Toxicol. Appl. Pharmacol. 1972, **23**, 288.
3. Sax, N. I. et al *Dangerous Properties of Industrial Materials* 7th ed., 1989, Van Nostrand Reinhold, New York, NY, USA.
4. IARC Monograph 1987, **Suppl. 7**, 73.
5. Chistyakov, V. V. et al *Khim. Farm. Zh.* 1988, **22**(10), 1158-1162 (Russ.) (*Chem. Abstr.* **10**, 689213v).
6. IARC Monograph 1975, **9**, 75.
7. Stokes, J. B. et al *Agric. Res. Results* 1981, 1-7.
8. Graf, U. et al *Mutat. Res.* 1989, **222**(4), 359-373.
9. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T347 tris(1-aziridinyl)phosphine sulfide



C₆H₁₂N₃PS

Mol. Wt. 189.22

CAS Registry No. 52-24-4

Synonyms triethylenethiophosphoramidate; *N,N'*-triethylenethiophosphamide; *N,N',N''*-tri-1,2-ethanediyolphosphorothioic triamide; thio-TEPA

EINECS No. 200-135-7

RTECS No. SZ 2975000

Uses Antineoplastic agent given orally or by injection.

Physical properties

M. Pt. 51.5°C

Solubility Water: 190 g l⁻¹ at 25°C. Organic solvents: benzene, chloroform, diethyl ether, ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird 5.62 mg kg⁻¹ (1).

LD₅₀ oral starling 17.8 mg kg⁻¹ (1).

LD₅₀ oral quail 237 mg kg⁻¹ (1).

LD₅₀ oral mouse 38 mg kg⁻¹ (2).

LD₅₀ intravenous rat 9-15 mg kg⁻¹ (3,4).

LD₅₀ intraperitoneal mouse 400 mg kg⁻¹ (5).

The oral LD₅₀ in mice is reduced if phenobarbitone is administered concomitantly (6).

Carcinogenicity and chronic effects

Inadequate evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2A (7).

National Toxicology Program tested rats and mice via intraperitoneal injection. Positive evidence of carcinogenicity was seen in rats and mice of both sexes (8).

National Toxicology Program classification: reasonably anticipated to be a human carcinogen (9).

Target organs for carcinogenicity: skin and the haematopoietic system in rats and mice and the preputial gland in mice (10).

Mice receiving 100 μmol kg⁻¹ by intraperitoneal injection for 8 wk and killed at 24 wk demonstrated a significant number of primary lung tumours (11).

Rats receiving 7% of the LD₅₀ by intravenous injection once weekly for 52 wk developed a significant number of malignant tumours (12).

Tested positive in the initiator tRNA acceptance assay for carcinogens (13).

Teratogenicity and reproductive effects

♂ Mice receiving doses 0.1-0.5 × LD₅₀ showed signs of testicular cytotoxicity which could be prevented by analogues of gonadotrophin-releasing hormone (14).

Pregnant mice injected intraperitoneally with single doses of 0.5-30 mg kg⁻¹ on various days of gestation showed signs of teratogenicity at doses >1 mg kg⁻¹. The malformations observed were exencephaly, spina bifida, cleft palate, kinky tail and digit alterations (15).

Pregnant rats receiving 5 mg kg⁻¹ developed foetuses with developmental abnormalities and skeletal defects (16).

Metabolism and toxicokinetics

In humans absorption from the gastro-intestinal tract is unreliable and incomplete. Absorption is also unreliable from intramuscular or intravenous injection sites, but it may be given by all parenteral routes (17,18). It can be absorbed through mucous membranes such as bladder and pleura (17). The primary metabolite is triethylenephosphoramidate (3,19) and further metabolism to aziridine occurs (20). Only traces of unchanged compound are excreted in urine (17), although species variation is seen (21).

Irritancy

Human skin and mucous membrane irritant (15).

Genotoxicity

Salmonella typhimurium TA100 without metabolic activation positive (22).

In vitro chromosomal aberrations in lymphocytes without metabolic activation positive (23).

Drosophila melanogaster DNA lesions positive (24).

Drosophila melanogaster (*w/w+*) eye mosaic assay positive (5mm) (25).

Other effects

Other adverse effects (human)

The compound is very toxic to the haemopoietic system, with maximum depression of the bone marrow occurring up to 30 days after therapy. Gastro-intestinal disturbances, headache, dizziness, hypersensitivity and impaired fertility have also been reported (17).

Any other adverse effects

Thio-TEPA caused a dose-dependent inhibition of the growth of P388 murine leukaemia cells in culture (26).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Substances extractable in chloroform guide level 0.1 mg l⁻¹ dry residue (27).

Other comments

Alkylating agent which can interact with DNA *in vitro* (4,19,20) and *in vivo* (17).

At temperatures above 2-8°C, thio-TEPA polymerises (28).

Toxicology, mutagenicity and carcinogenicity have been reviewed (28-30).

References

1. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
2. Giller, S. A. (Ed) *Imifos* 1968, 129, Riga, USSR.
3. Boone, I. U. *Toxicol. Appl. Pharmacol.* 1962, **4**, 344-353.
4. Scherf, et al *Arzneim.-Forsch.* 1970, **20**, 1467.
5. Munson, A. E. et al *Pharmacology* 1974, **11**, 231-240.
6. Bruce, et al *Can. J. Genet. Cytol.* 1979, **21**, 319-334.
7. IARC Monograph 1987, **Suppl. 7**, 368.
8. *National Toxicology Program Research and Testing Division* 1996, Report No. TR-058, NIEHS, Research Triangle Park, NC, USA.
9. *Eighth Report on Carcinogens* 1998, National Toxicology Program, NIEHS, Research Triangle Park, NC 27709, USA.
10. Swirsky-Gold, L. *Mutat. Res.* 1993, **283**, 75-100.
11. Stoner, G. D. et al *Cancer Res.* 1973, **33**, 3069-3085.
12. Schmahl, D. et al *Arzneim.-Forsch.* 1970, **20**, 1461-1467.
13. Hradec, J. *Carcinogenesis (London)* 1989, **10** (8), 1413-1417.
14. Kim, S. W. *K'at'ollik Taehak Uliha kpu Nonmunjip* 1989, **42** (3), 723-733.
15. Tanimura, T. *Okajimas Folia Anat. Jpn.* 1968, **44**, 203-253.
16. Murphy, M. L. et al *Ann. N. Y. Acad. Sci.* 1958, **68**, 762-782.
17. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.

18. Bateman, J. L. et al *Int. J. Appl. Radiat.* 1960, **7**, 287-298.
19. Cohen, N. A. *Cancer Res.* 1991, **51** (16), 4360-4366.
20. Egorin, M. J. et al *Cancer Res.* 1990, **50** (13), 4044-4049.
21. Craig, A. N. et al *Biochem. Pharmacol.* 1959, **3**, 42-50.
22. Zeiger, E. et al *Environ. Mol. Mutagen.* 1992, **19**, 2-14.
23. Yakavenko, K. N. et al *Cytol. Genet.* 1982, **16**, 55-59.
24. Vogel, E. W. *Mutat. Res.* 1989, **211** (1), 153-170.
25. Vogel, W. V. et al *Mutagenesis* 1993, **8**(1), 57-81.
26. Miller, B. et al *Cancer Lett.* 1988, **41**, 157-168.
27. EC Directive relating to the Quality of Water Intended for Human Consumption 1982, 80/77/8EEC, Office for Official Publications of the European Communities, 2, rue Mercier, L-2985 Luxembourg.
28. IARC Monograph 1990, **50**, 123-141.
29. IARC Monograph 1987, **Suppl. 6**, 549.
30. IARC Monograph 1975, **9**, 85-94

T348 tris(2-butoxyethanol) phosphate



$\text{C}_{18}\text{H}_{39}\text{O}_7\text{P}$

Mol. Wt. 398.48

CAS Registry No. 78-51-3

Synonyms KP 140; tri(2-butoxyethanol phosphate); tributyl cellosolve phosphate; TBEP; tributoxyethyl phosphate; 2-butoxyethanol phosphate

EINECS No. 201-122-9

RTECS No. KJ 9800000

Uses Plasticiser.

Physical properties

M. Pt. -70°C **B. Pt.** 215-228°C at 4 mmHg **Flash point** 224°C **Specific gravity** 1.02 at 20°C with respect to water at 20°C **Volatility** v.p. 0.03 mmHg at 150°C; v.den. 13.8

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, guinea pig 3000 mg kg⁻¹ (1,2).

LD₅₀ intravenous mouse 180 mg kg⁻¹ (3).

Sub-acute and sub-chronic data

Gavage Sprague Dawley rats (18 wk) 0.25-0.5 ml kg day⁻¹ 5 day wk⁻¹ caused neurotoxicity (4-6).

Irritancy

Dermal rabbit (24 hr) 500 mg caused mild irritation and 500 mg instilled into rabbit eye caused mild irritation (7).

Other effects

Other adverse effects (human)

Detected in human adipose tissue, 25-483 µg g⁻¹ in Canada (8).

Interacts with β-adrenergic transport proteins, β-adrenergic receptors coupled to adenylate cyclase and with non-specific tissue binding sites. May alter catecholamine-sensitive adenylate cyclase activity (9).

Other comments

Contaminant in tap water in Japan, 0 to 58.5 ppt detected over the period of 1 yr (10).

Fish and shellfish captured in Okayama Prefecture Japan contained <0.005-0.019 µg g⁻¹ (11).
Reviews on experimental toxicology and human health effects listed (12).

References

1. *Raw Mater. Data Handbook* 1975, **2**, 93.
2. LeFaux, R. *Prac. Toxicol. Plastics* 1968, 336.
3. *US Army Armament Res. Develop. Command.*
4. Laham, S. et al *J. Appl. Toxicol.* 1984, **4**(1), 42-48.
5. Laham, S. et al *Am. Ind. Hyg. Assoc.* 1985, **8**, 442-448.
6. Laham, S. et al *Chemosphere* 1984, **13**(7), 801-812.
7. *Prehled Prumyslove Toxikol Org Latky* 1986, 1142.
8. Le Bel, G. L. et al *Bull. Environ. Contam. Toxicol.* 1989, **43**(2), 225-230.
9. Sager, G. et al *Biochem. Pharmacol.* 1989, **38**(15), 2551-2557.
10. Adachi, K. et al *Hyogo-ken Eisei Kenkyusho Kenkyu Hokoku* 1984, **19**(1-6), (Jap.) (*Chem. Abstr.* **103**, 11048t).
11. Kenmochi, V. et al *Okayama-Ken Kankyo Hoken Senta Nenpo* 1981, (5), 167-175, (Jap.) (*Chem. Abstr.* **99**, 68978z).
12. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T349 tris(2-chloroethyl)amine



C₆H₁₂Cl₃N

Mol. Wt. 204.53

CAS Registry No. 555-77-1

Synonyms 2,2',2''-trichlorotriethylamine; 2-chloro-*N,N*-bis(2-chloroethyl)ethanamine; tris(β-chloroethyl)-amine

RTECS No. YE 2625000

Uses Antineoplastic agent, as hydrochloride.

Physical properties

M. Pt. -4°C **B. Pt.** 144°C at 15 mmHg **Specific gravity** 1.2347 at 25°C with respect to water at 4°C

Solubility Organic solvents: miscible with carbon tetrachloride, dimethylformamide

Environmental fate

Abiotic removal

Can be detoxified with pyrophoric metallic powder followed by thermal pyrolysis and deflagration (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral blackbird, quail 31.6, 117-133 mg kg⁻¹, respectively (2).

LD₅₀ oral quail 133 mg kg⁻¹ (3).

LD₅₀ oral rat 5 mg kg⁻¹ (4).

LC₅₀ (10 min) inhalation rat 200 mg m⁻³ (5).

LD₅₀ dermal rat, dog 2, 10 mg kg⁻¹, respectively (4).

Irritancy

Compound is a necrotising irritant (6).

Other effects

Other adverse effects (human)

In vitro Chinese hamster V79 cells without metabolic activation positive (7).

In vitro human EVE cells inhibition of DNA synthesis without metabolic activation positive (7).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorines: guide level 1 µg l⁻¹ (8).

Included in Schedule 6 (Release into the Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (9).

Other comments

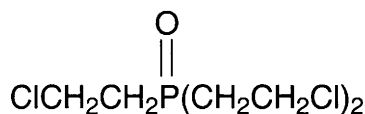
Can persist in water after dechlorination (10).

Alkylating agent, but with little effect on proteins in cell membranes of humans erythrocytes or L5178Y cells (11).

References

1. Sayles, D. C. *U S* 41949,641 Appl. 488,545, 5 Mar 1990.
2. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
3. *J. Reprod. Fertil.* 1976, **48**, 371.
4. *NTIS Report* PB158-507, Natl. Tech. Inf. Ser., Springfield, VA, USA.
5. *NTIS Report* PB158-508, Natl. Tech. Inf. Ser., Springfield, VA, USA.
6. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
7. Slamenova, D. et al *Neoplasma* 1986, **33**(6), 699-706.
8. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
9. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
10. Tingfa, D. et al *Water, Air, Soil Pollut.* 1990, **49**(1-2), 63-67.
11. Ankel, E. G. et al *Int. J. Tissue React.* 1986, **8**(5), 347-354

T350 tris(2-chloroethyl) phosphate



C₆H₁₂Cl₃O₄P

Mol. Wt. 285.49

CAS Registry No. 115-96-8

Synonyms 2-chloro-ethanol, phosphate (3:1); tris(β-chloroethyl) phosphate; Niaux 3CF; Genomol P; Cellulflex CEF

EINECS No. 204-118-5

RTECS No. KK 2450000

Uses Flame retardant plasticiser.

Physical properties

M. Pt. 192°C at 10 mmHg **Flash point** 232°C **Volatility** v.p. 0.5 mmHg at 145°C

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed – Irritating to eyes and skin (R22, R36/38)

Safety phrases Keep out of reach of children (if sold to general public) (S2)

Ecotoxicity

Bioaccumulation

Confirmed to be non or low accumulative (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1230 mg kg⁻¹ (2).

Sub-acute and sub-chronic data

Gavage rats, mice (16 day) 22-350, 44-700 mg kg⁻¹, respectively. No chemical-related deaths, differences in mean body-weight or histopathological lesions were observed. Serum cholinesterase activity was reduced slightly in ♀ rats receiving 175 or 350 mg kg⁻¹ (3).

Gavage rats, mice (16 wk) 22-350, 44-700 mg kg⁻¹, respectively. No chemical-related deaths, differences in mean body-weight or differences in cholinesterase activity were observed in mice. Several rats receiving 175 or 350 mg kg⁻¹ died from chemical toxicity. Chemical-related neuronal necrosis occurred in the hippocampus and thalamus of ♀ rats and, to a lesser extent, in ♂ rats. Final mean body-weights of ♀ rats receiving 350 mg kg⁻¹ were 20% greater than those of controls. Serum cholinesterase activity was reduced in ♀ receiving 175 and 350 mg kg⁻¹ (3).

Carcinogenicity and chronic effects

National Toxicology Program tested rats and mice via gavage. Clear evidence of carcinogenicity (increased incidence of dose-related malignant and benign neoplasm) in ♂ and ♀ rats, equivocal evidence in ♂ and ♀ mice (3).

Gavage rats (2 yr) 0, 44 or 88 mg kg⁻¹ 5 × wk⁻¹ for 104 wk. The survival of ♂ and ♀ rats given the highest dose was reduced relative to controls. Focal hyperplasia of the renal tubule epithelium and renal tubule adenomas were significantly increased in ♂ rats given 88 mg kg⁻¹ and, to a lesser extent, in ♀ rats. Gliosis, haemorrhage, pigmentation and mineralisation were observed in the brains of >50% of ♀ rats receiving 44 or 88 mg kg⁻¹ (3). Gavage mice (2 yr) 0, 175 or 350 mg kg⁻¹ 5 × wk⁻¹ for 104 wk. Nuclear enlargement of tubule epithelial cells in the kidney was seen in ~80% of high-dose mice. Treated ♀ mice also showed a slight increase in the incidence of neoplasms of the Harderian gland (3).

Teratogenicity and reproductive effects

Gavage mice (13 wk) 44, 175, 700 mg kg⁻¹ reduced epididymis and testis weight. No effect on body weight or cauda epididymis weight. An increase in % abnormal sperm, but no effect on sperm motility (4).

Gavage rat (13 wk) 22, 88, 175 mg kg⁻¹ reduced sperm motility. No effect on % abnormal sperm, weights of reproductive organs or body weight (4).

Metabolism and toxicokinetics

Following an oral dose to mice and rats of 175 mg kg⁻¹ radiolabelled compound, mice eliminated >70% of radioactivity in 8 hr while rats eliminated only 40%; the metabolic profile of radioactivity in urine was similar for both species. The major metabolite found in ♀ rat urine was bis(2-chloroethyl)carboxymethyl phosphate; two additional metabolites were identified as bis(2-chloroethyl) hydrogen phosphate and the glucuronide of bis(2-chloroethyl) 2-hydroxyethyl phosphate (5).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (3).

In vitro Chinese hamster ovary cells chromosomal aberrations negative; an equivocal response was produced with metabolic activation for the induction of sister chromatid exchanges (3).

In vitro Chinese hamster ovary cells with and without metabolic activation chromosomal aberrations negative; with metabolic activation a slight increase in sister chromatid exchanges was seen in 1 of 2 tests (6).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level 1 µg l⁻¹. Phosphorus: guide level 400 µg l⁻¹, maximum admissible concentration 5000 µg l⁻¹ (both as P₂O₅) (7).

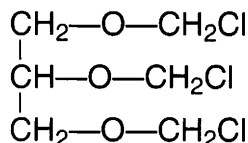
Other comments

Human health effects, experimental toxicology, physico-chemical properties, ecotoxicology, environmental effects, exposure levels, workplace experience reviewed (8,9).

References

1. *The list of existing chemical Substances tested on biodegradability by microorganism or bioaccumulation in fish body* 1987, Chemicals Inspection and Testing Institute, Japan.
2. *Bull. Environ. Contam. Toxicol.* 1977, **17**, 77.
3. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-391, NIEHS, Research Triangle Park, NC, USA.
4. Morrissey, R. E. et al *Fundam. Appl. Toxicol.* 1988, **11**(2), 343-358.
5. Burka, L. T. et al *Drug Metab. Dispos.* 1991, **19**(2), 443-447.
6. Galloway, S. M. et al *Environ. Mol. Mutagen.* 1987, **10**(Suppl. 10), 1-175.
7. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
8. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
9. *BIBRA Toxicity Profile* 1988, British Industrial Biological Research Association, Carshalton, UK

T351 1,2,3-tris(chloromethoxy)propane



C₆H₁₁Cl₃O₃

Mol. Wt. 237.51

CAS Registry No. 38571-73-2

Synonyms glycerol tris(chloromethyl) ether

RTECS No. UA 1850000

Physical properties

Specific gravity 1.3575 at 17.5°C with respect to water at 4°C (1)

Mammalian & avian toxicity

Carcinogenicity and chronic effects

No adequate data for carcinogenicity to humans, limited evidence for carcinogenicity to animals, IARC classification group 3 (2).

Dermal ♀ ICR/Ha Swiss mice (6-8 wk old) 1 mg on the dorsal skin 3 times wk⁻¹ for up to 502 days. 6/50 mice developed skin papillomas and 3/50 had local squamous-cell carcinomas. No skin tumours were observed in the control group. Subcutaneous injection of 0.3 mg in 0.05 ml tricapyrin once a week for 569 days resulted in 12/50 mice with malignant tumours at the injection site. In the control group injected with tricapyrin alone, no local tumours occurred. Intraperitoneal injection of 0.3 mg in 0.05 ml tricapyrin once a week for 532 days caused local sarcomas in 5/30 mice. In 30 controls injected with tricapyrin alone, no local malignant tumours occurred (3).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level 1 $\mu\text{g l}^{-1}$ (4).

Included in Schedule 6 (Release into Land: Prescribed Substances) of Statutory Instrument No. 472, 1991 (5).

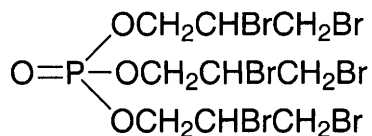
Other comments

Human health effects and experimental toxicology reviewed (6).

References

1. Lichtenberger, J. et al *Bull. Soc. Chim. Fr.* 1947, **14**, 468-476.
2. *IARC Monograph* 1987, **Suppl. 7**, 73.
3. Van Duuren, B. L. et al *Cancer Res.* 1975, **35**, 2553-2557.
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
5. *S.I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
6. *IARC Monograph* 1977, **15**, 301

T352 tris(2,3-dibromopropyl) phosphate



$\text{C}_9\text{H}_{15}\text{Br}_6\text{O}_4\text{P}$

Mol. Wt. 697.61

CAS Registry No. 126-72-7

Synonyms phosphoric acid, 2,3-dibromopropyl ester; 2,3-dibromo-1-propanol, phosphate (3:1); Tris-BP; Flammex AP; Firemaster T23P; Fyrol HB32

EINECS No. 204-799-9

RTECS No. UB 0350000

Uses Flame retardant.

Physical properties

M. Pt. 5.5°C Flash point >112°C Specific gravity 2.27 at 25°C

Environmental fate

Degradation studies

Degradation by organisms such as *Acinetobacter calcoaceticus* has been compared with that achieved by activated sludge (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1010 mg kg⁻¹ (2).

LD₅₀ intraperitoneal mouse 300 mg kg⁻¹ (3).

LD₅₀ dermal rabbit >8 g kg⁻¹ (4).

Sub-acute and sub-chronic data

Single oral doses in the range 25-200 mg kg⁻¹ and repeated in the range 50-200 mg kg⁻¹ for 7 days produced nephrotoxic effects in rats. Desquamation and necrosis of kidney tubular cells were seen along with increased urinary levels of glucose, lactate, γ -glutamyl transferase and lactate dehydrogenase activities (5).

Carcinogenicity and chronic effects

Limited evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2A (6).

National Toxicology Program tested rats and mice via feed. Positive evidence of carcinogenicity was seen in both species in both sexes (7,8). σ and φ mice receiving the compound for 103 wk in diet showed an increased incidence of tumours, particularly squamous cell carcinomas and papillomas of the forestomach and carcinomas of the lung. Renal damage was also seen (8).

In the study with rats, the compound increased the incidence of renal tubular cell adenomas in both sexes (8).

Mice receiving the compound dermally twice weekly for ≥ 496 days developed tumours of skin, lung, forestomach and oral cavity (9).

Teratogenicity and reproductive effects

σ Rabbits painted with 2.27 g kg⁻¹ on intact or abraded skin once wkly for 3 month showed a reduction in testicular weight and abnormality of spermatogenesis (10).

Metabolism and toxicokinetics

The compound is absorbed from the gastro-intestinal tract and through skin in a dose-dependent manner (11).

Bromine can be detected in muscle, liver and fat after repeated administration (12).

A metabolic hydrolysis product 2,3-dibromopropanol has been detected in free and conjugated form in urine from rat following skin application of 100 mg rat⁻¹ (13).

Rabbits treated by application to clipped skin of fabric dipped in the compound absorbed up to 17% over 96 hr (14).

Irritancy

Compound is non-irritant to rabbit skin or eye (11,12).

Sensitisation

No evidence of skin sensitisation has been seen in guinea pigs (15).

Genotoxicity

Salmonella typhimurium TA100 with metabolic activation positive, without metabolic activation negative (16).

In vitro unscheduled DNA synthesis in primary hepatocytes weak positive (17).

In vitro Chinese hamster V79 cells without metabolic activation chromosomal aberrations negative (18).

Drosophila melanogaster sex linked recessive lethals in σ germ-cell stages positive (19).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (20).

Other comments

Uses, metabolism, mutagenicity and organ damage have been reviewed (21).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (22).

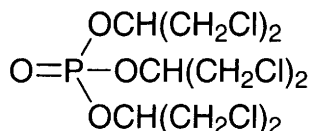
Toxicology and mutagenicity reviewed (4,23).

References

1. Heymann, J. B. et al *Water Sci. Technol.* 1989 **21**(4-5), 397-408.
2. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
3. *NTIS Report No. AD277-689 Natl. Tech. Inf. Ser.*, Springfield, VA, USA.
4. *IARC Monograph* 1979, **20**, 575.
5. Fukuoka, M. et al *J. Appl. Toxicol.* 1987 **7**(1), 23-34.

6. IARC Monograph 1987, **Suppl. 7**, 369.
7. National Toxicology Program Research and Testing Division 1992, Report No. TR-076, NIEHS, Research Triangle Park, NC, USA.
8. National Cancer Institute 1978, NIH 78-1326 (TR-076).
9. Van Duuren, B. L. et al *Cancer Res.* 1978, **38**, 3236-3240.
10. Dybing, E. et al *Rev. Biochem. Toxicol.* 1989, **10**, 139-86.
11. Daniher, F. A. *Proc. Symp. Textile Flammability* 1976, **4**, 126-143.
12. Kerst, A. F. J. *Fire Flamm. Fire Retard. Chem.* 1974, **1**, 205-217.
13. St John, L. E. *Bull. Environ. Contam. Toxicol.* 1976, **15**, 192-197.
14. Alsamer, A. G. et al *J. Environ. Pathol. Toxicol.* 1978 **1**, 543-549.
15. Morrow, R. W. et al *Am. Ind. Hyg. Assoc. J.* 1976, **37**, 192-197.
16. Distlerath *Mutat. Res.* 1984, **136**, 55-64.
17. Gordon et al *Carcinogenesis (London)* 1985, **6**, 705.
18. Furukawa, M. et al *J. Natl. Cancer Res.* 1978, **60**, 1179-1181.
19. Valencia, R. IX Annual Meeting of American Environmental Mutation Society 1978, San Fransisco, CA, USA.
20. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
21. Osterberg, R. E. et al *J. Toxicol. Environ. Health* 1977, **3**, 979-987.
22. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
23. IARC Monograph 1987, **Suppl. 6**, 554

T353 tris(1,3-dichloro-2-propyl) phosphate



$\text{C}_9\text{H}_{15}\text{Cl}_6\text{O}_4\text{P}$

Mol. Wt. 430.91

CAS Registry No. 13674-87-8

Synonyms Fyrol FR-2

EINECS No. 237-159-2

RTECS No. UB 1473000

Uses Flame retardant.

Physical properties

B. Pt. 236-237°C at 5 mmHg

Solubility Water: ~100mg l⁻¹

Environmental fate

Degradation studies

When present in river water it can be rapidly degraded by bacteria, apparently using the compound as a carbon source (species unspecified) (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1.85 g kg⁻¹ (2).

LD₅₀ oral ♂ mouse 2.67 g kg⁻¹, ♀ mouse 2.25 g kg⁻¹ (3).

Toxic symptoms in mice included ataxia, hyperactivity and convulsions (3).

Sub-acute and sub-chronic data

Mice fed 0.01-1.33% in diet for 3 months yielded a NOEC of 0.01% diet.

All animals fed 1.33% diet died within one month and those receiving $\geq 0.13\%$ diet showed raised serum levels of alkaline phosphatase and alanine aminotransferase activities (3).

Teratogenicity and reproductive effects

Oral ♀ pregnant rats (7-15 day of gestation) 25-400 mg kg⁻¹. A marked suppression of maternal body weight gain and food consumption was seen in rats administered 200 and 400 mg kg⁻¹. An increase in foetal death was observed in rats given 400 mg kg⁻¹, but no increase in the incidence of gross and visceral malformations was seen. No effects on offspring were observed. Thus the compound is considered not to have a teratogenic effect but did elicit maternal toxicity at 200-400 mg kg⁻¹ (4).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC Organochlorine compounds: guide level 1 µg l⁻¹ (5).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (6).

Other comments

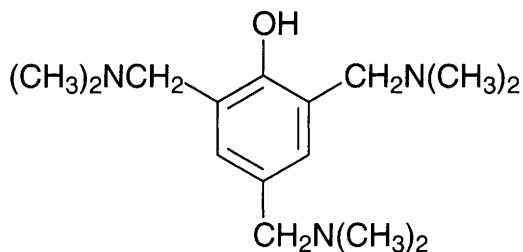
Reviews on human health effects, experimental toxicology, physico-chemical properties listed (7).

Toxicity has been reviewed.

References

1. Kawai, S. et al *Annu. Rep. Osaka City Inst. Public Health Environ. Sci.* 1985, **48**, 175-183.
2. *Bromatol. Chem. Toksykol.* 1976, **9**, 141.
3. Kamata, E. et al *Eisei Shikensho Hokoku* 1989, **107**, 36-43 (Japan).
4. *J. Toxicol. Sci.* 1983, **8**, 339.
5. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
6. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
7. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T354 2,4,6-tris(dimethylaminomethyl)phenol



$C_{15}H_{27}N_3O$

Mol. Wt. 265.40

CAS Registry No. 90-72-2

Synonyms 2,4,6-tri[(dimethylamino)methyl]phenol

EINECS No. 202-013-9

RTECS No. SN 3500000

Uses Accelerator for epoxy resin cross-linkage.

Physical properties

B. Pt. 130-135°C at 1 mmHg Flash point >110°C Specific gravity 0.969

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed – Irritating to eyes and skin (R22, R36/38)

Safety phrases Keep out of reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – After contact with skin, wash immediately with plenty of water (S2, S26, S28)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1.2 g kg⁻¹ (1).

LD₅₀ dermal rat 1.28 g kg⁻¹ (2).

Irritancy

Dermal rabbit (24 hr) 500 mg and 50 µg instilled into rabbit eye caused severe irritation (3).

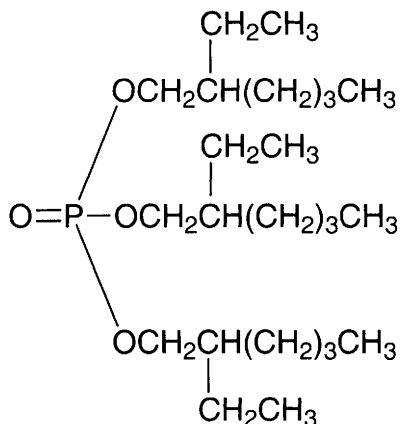
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (4).

References

1. *Russian Pharmacol. Toxicokol.* 1974, **3**, 130.
2. *Data Sheets* Rohm & Haas Co., Philadelphia, PA, USA.
3. Marhold, J. V. *Sbornik Vysledku Toxilogickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
4. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T355 tris(2-ethylhexyl) phosphate



$\text{C}_{24}\text{H}_{51}\text{O}_4\text{P}$

Mol. Wt. 434.64

CAS Registry No. 78-42-2

Synonyms phosphoric acid, tris(2-ethylhexyl) ester; triethylhexyl phosphate; tri-*sec*-octyl phosphate; 2-ethyl-1-hexanol phosphate; Disflamoll tof; Tof

EINECS No. 200-116-6

RTECS No. MP 0770000

Uses Flame retardant.

Physical properties

M. Pt. -74°C B. Pt. 216° at 5 mmHg Flash point $>110^{\circ}\text{C}$ Specific gravity 0.9262 at 20°C with respect to water at 20°C Volatility v.den. 14.95

Environmental fate

Degradation studies

The compound can be degraded by bacteria collected from river water that appear to use the compound as a carbon source (species unspecified) (1,2).

Mammalian & avian toxicity

Acute data

LD_{50} oral rat 37 g kg^{-1} (3).

LD_{50} dermal rabbit 20 g kg^{-1} (4).

Carcinogenicity and chronic effects

National Toxicology Program tested rats and mice via gavage. Equivocal evidence for carcinogenicity was seen in ♂ rats, no evidence for carcinogenicity in ♀ rats or ♂ mice and some evidence for carcinogenicity in ♀ mice (5,6). Liver carcinomas were seen in ♀ mice (6).

Irritancy

Moderate irritation was caused by 100 mg applied to rabbit eye or 250 mg applied to rabbit skin (4).

Other comments

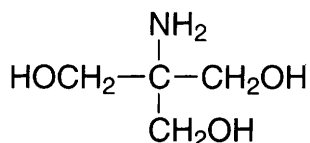
Reviews on human health effects, experimental toxicology, physico-chemical properties listed (7).

The risk of carcinogenicity based on *Salmonella typhimurium* mutagenicity results has been assessed (8).

References

1. Kawai, S. et al *Annu. Rep. Osaka City Inst. Public Health Environ. Sci.* 1985, **48**, 175-183.
2. Kawai, S. et al *Annu. Rep. Osaka City Inst. Public Health Environ. Sci.* 1986, **49**, 160-166.
3. *J. Ind. Hyg. Toxicol.* 1948, **30**, 63.
4. Deichmann, W. B. *Toxicology of Drugs and Chemicals* 1969, Academic Press, New York, NY, USA.
5. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-274, NIEHS, Research Triangle Park, NC, USA.
6. Zeiger, E. *Cancer Res.* 1987, **47**(5), 1287-1296.
7. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium.
8. Benigni, R. *Mutat. Res.* 1990 **244**(1), 79-91

T356 tris(hydroxymethyl)aminomethane



$\text{C}_4\text{H}_{11}\text{NO}_3$

Mol. Wt. 121.14

CAS Registry No. 77-86-1

Synonyms trimethanamine; 2-amino-2-(hydroxymethyl)-1,3-propanediol; trimethylaminomethane; trisamine; Trometamol; trisbuffer; Tham

EINECS No. 201-064-4

RTECS No. TY 2900000

Uses As a laboratory buffer and in pharmaceuticals, cosmetics and cleaning agents.

Physical properties

M. Pt. 171-172°C **B. Pt.** 219-220°C at 10 mmHg

Solubility Water: 550 g l⁻¹ at 25°C. Organic solvents: acetone, ethylene glycol, methanol

Ecotoxicity

Invertebrate toxicity

Causes low anionic cuticular permeability in shore crabs, which can interfere with ionic exchanges across the whole gill (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 5.9 g kg⁻¹ (2).

LD₅₀ oral rabbit 1 g kg⁻¹ (3).

LD₅₀ intravenous mouse 1.21 g kg⁻¹ (4).

Other effects

Other adverse effects (human)

Can cause intravascular irritation and tissue necrosis if improperly used in therapy (5-7).

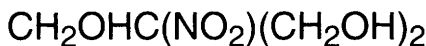
Other comments

The compound is an organic amine proton acceptor. It can be used clinically in the treatment of acidosis and to stabilise blood pH *ex vivo* (5).

References

1. Lignan, J. M. *J. Exp. Biol.* 1987, **131**, 159-174.
2. Bollett. *Chim. Farmac.* 1971, **110**, 653.
3. *J. Ind. Hyg. Toxicol.* 1940, **22**, 315.
4. *Acta Biol. Med. Germanica* 1966, **17**, 217.
5. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
6. Rehder, H. et al *Arch. Dis. Child.* 1974, **49**, 76.
7. Goldenburg, V. E. et al *J. Am. Med. Assoc.* 1968, **205**, 81-84

T357 tris(hydroxymethyl)nitromethane



C₄H₉NO₅

Mol. Wt. 151.12

CAS Registry No. 126-11-4

Synonyms 2-(hydroxymethyl)-2-nitro-1,3-propanediol; trimethylnitromethane; 2-nitro-2-(hydroxymethyl)-1,3-propanediol; trihydroxymethylnitromethane

EINECS No. 204-769-5

RTECS No. TY 7350000

Uses Bactericide for industrial water systems, cutting oils, nonprotein glues and sizings.

Physical properties

M. Pt. 214°C (pure)

Solubility Water: 2.2 g ml⁻¹ at 20°C. Organic solvents: ethanol

Ecotoxicity

Invertebrate toxicity

EC₅₀ (5-30 min) *Photobacterium phosphoreum* 2.34 ppm Microtox test (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 1900 mg kg⁻¹ (2,3).

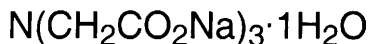
LD_{Lo} oral rabbit 250 mg kg⁻¹ (4).

LD₅₀ intraperitoneal mouse 4000 mg kg⁻¹ (5).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
2. *Ind. Med. Surg.* 1970, **39**, 56.
3. *Pesticide Chemicals Official Compendium* 1966, Assoc. Am. Pest. Contr. Officials, KS, USA.
4. *J. Ind. Hyg. Toxicol.* 1940, **22**, 315.
5. *Khim. Zhizn* 1977, **11**(1), 73

T358 trisodium nitrilotriacetate, monohydrate



$\text{C}_6\text{H}_8\text{NO}_7\text{Na}_3$

Mol. Wt. 275.10

CAS Registry No. 18662-53-8

Synonyms NTA sodium hydrate; *N,N*-bis(carboxymethyl)glycine trisodium salt monohydrate

RTECS No. AJ 1070000

Uses In detergents and in indium plating.

Physical properties

M. Pt. >300°C

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) rainbow trout, scud 98 mg l⁻¹; fathead minnow 127 mg l⁻¹, bluegill sunfish 253-487 mg l⁻¹; scup 3105 mg l⁻¹, mummichog 5500 mg l⁻¹ (1).

Invertebrate toxicity

LC₅₀ (96, 168 hr) grass shrimp 4.1, 1.8 g l⁻¹, respectively (1).

LC₅₀ (96, 168 hr) hermit crab 5.5 g l⁻¹, 1.8 g l⁻¹, respectively (1).

LC₅₀ (96, 168 hr) *Mytilus edulis* 6.1 g l⁻¹, 3.4 g l⁻¹, respectively (1).

LC₅₀ (96, 168 hr) *Mercenaria mercenaria* >10 g l⁻¹ (1).

Environmental fate

Degradation studies

No evidence of detrimental effects to efficiency of activated sludge biomass at 20 mg l⁻¹ carbon (2).

Degrades via: iminodiacetic acid; glycine; ammonia; glyoxylate; and glycerate (3).

Readily mineralised by microorganisms under aerobic and denitrifying conditions, and there is no evidence of formation of toxic metabolites; significant mobilisation and transport of trace metals by nitrilotriacetic acid from river sediments to groundwater is unlikely, and groundwater contamination from infiltrating river water is unlikely to cause severe problems under environmental conditions at 0.9-1.1 mg l⁻¹ (4).

Biodegradability of nitrilotriacetic acid increases with temperature, with 3% removal at 5°C and 98% removal at 20°C of an initial concentration of 5-20 mg l⁻¹ (5).

Up to 97% nitrilotriacetic acid was biologically degraded in a sewage treatment plant; average daily load was 13 kg nitrilotriacetic acid day⁻¹, influent concentration 300-1500 µg l⁻¹ nitrilotriacetic acid (6).

Removal of nitrilotriacetic acid during wastewater treatment at three activated sludge plants averaged 91% (7).

Mammalian & avian toxicity

Carcinogenicity and chronic effects

National Toxicology Program tested rats and mice via feed at 2% for 2 yr. Clear evidence of carcinogenesis in both species, producing kidney and bladder neoplasms (8,9).

The liver and kidney toxicity may be due to nitrilotriacetic acid chelating activity (9).

Teratogenicity and reproductive effects

Administered at 0.1-20 mg kg⁻¹ in drinking water on days 6-14 of pregnancy, it did not enhance teratogenicity of cadmium chloride or methyl mercury in rats (10).

Metabolism and toxicokinetics

Nitrilotriacetic acid is not biotransformed and is excreted almost entirely unchanged in urine of rats and mice (9).

Genotoxicity

Induced diptheria toxin-resistant (DTR) mutants in human cell line EUE (11).

Legislation

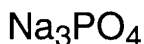
Drinking Water Limit in The Netherlands for nitrilotriacetic acid 4 µg l⁻¹ (12).

Drinking Water Limit in Switzerland for nitrilotriacetic acid 3 µg l⁻¹, and in Canada 50 µg l⁻¹ (based on non-genotoxic risk assessment).

References

1. *An evaluation of the toxicity of nitrilotriacetic acid to marine organisms* 1970, Natl. Marine Water Qual. Lab.
2. *Environmental Effect of Photoprocessing Chemicals* 1974, Natl. Assoc. Photog. Manuf.
3. Van Echteld, C. J. A. et al *H₂O* 1978.
4. Kuhn, E. et al *Water Res.* 1987, **21**(10), 1237.
5. Prakash, A. *NTA – An Ecological Appraisal* NRCC No. 15023, ISSN 03160114.
6. Siegrist, H. *Gas, Wasser, Abwasser* 1988, **68**(3), 101.
7. Wendt, R. H. et al *Environ. Toxicol. Chem.* 1988, **7**, 275.
8. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-677, NIEHS, Research Triangle Park, NC, USA.
9. Anderson, R. L. et al *CRC, Crit. Rev. Toxicol.* 1985, **15**, 1-102.
10. Nolen, G. A. et al *Toxicol. Appl. Pharmacol.* 1972, **23**, 222-37.
11. Grilli, M. P. et al *Toxicol. Lett.* 1985, **25**, 137-141.
12. Kanowski, S. *Das NTA – Problems in Organic Micropollutants in the Aquatic Environment*, Angeletti, G. et al (Eds.) Reidel, The Netherlands

T359 trisodium phosphate



$\text{Na}_3\text{O}_4\text{P}$

Mol. Wt. 163.94

CAS Registry No. 7601-54-9

Synonyms sodium phosphate, tribasic; trisodium orthophosphate; phosphoric acid, sodium salt (1:3)

EINECS No. 231-558-5

RTECS No. TC 9490000

Uses In photographic developers. Clarifying sugar. Water softener. In paper manufacture, laundering and tanning leather. In detergents.

Physical properties

Specific gravity 2.536 at 17.5°C

Solubility Water: 88 g l⁻¹

Mammalian & avian toxicity

Acute data

LD_{Lo} intravenous rabbit 1580 mg kg⁻¹ (1).

Metabolism and toxicokinetics

In humans, ~66% of ingested phosphate is absorbed from the gastro-intestinal tract; most is filtered by the glomeruli and partially resorbed. Absorption and resorption are stimulated by vitamin D and parathyroid hormone. Virtually all absorbed phosphate is eventually excreted via urine, and a small amount via faeces. The principal anion of extracellular fluid, it exists in the body as divalent (80%) and monovalent (20%) ions. It is

involved in many physiological processes, including carbohydrate and lipid metabolism, energy storage and transfer, formation of buffer systems and renal excretion of hydrogen ions. Normal plasma concentration is 0.8-1.5 mmol l⁻¹. Concentration of phosphate and calcium is inversely related (2).

Irritancy

Single 24 hr exposure to 2% is probably non-irritant for most humans as this concentration is recommended for diagnosing sensitisation (3).

Genotoxicity

Induced chromosome damage in *Drosophila melanogaster* (4).

Other effects

Other adverse effects (human)

Excess phosphate administration, particularly intravenously, may cause hyperphosphataemia, hypocalcaemia and ectopic calcification, hypotension, oedema and renal failure. Adverse effects are less common after oral administration but nausea, vomiting, diarrhoea and abdominal pain have been reported (2).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (5). Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phosphorus: guide level 400 µg l⁻¹; maximum admissible concentration 5000 µg l⁻¹ (as P₂O₅). Sodium: guide level 20 mg l⁻¹; maximum admissible concentration 150 mg l⁻¹ (6).

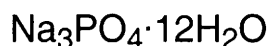
Other comments

UK reference nutrient intake 550 mg day⁻¹, US recommended daily allowance 800 mg day⁻¹ (2). Toxicity reviewed (7).

References

1. *Abderalden's Handbuch der Biologischen Arbeitsmethoden* 1935, Leipzig, Germany.
2. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
3. Fischer, A. A. *Contact Dermatitis* 2nd ed., 1973, Lea & Febiger, Philadelphia, PA, USA.
4. *Drosophila Information Service* 1946, 20, 87.
5. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
6. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
7. *BIBRA Toxicity Profile: phosphoric acid and its inorganic phosphates* 1987, British Industrial Biological Research Association, Carshalton, Surrey, UK

T360 trisodium phosphate dodecahydrate



H₂₄O₁₆Na₃P

Mol. Wt. 380.12

CAS Registry No. 10101-89-0

Synonyms sodium phosphate dodecahydrate

RTECS No. TC 9575000

Uses In photographic developers. Clarifying sugar. Removing boiler scales. Detergent mixtures. Softening water.

Physical properties

M. Pt. 75°C **Specific gravity** 1.62
Solubility Water: soluble in 3.5 parts water

Mammalian & avian toxicity

Acute data
LD₅₀ oral rat 7.4 g kg⁻¹ (1).

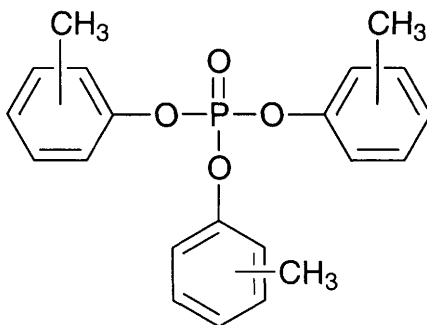
Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (2).
Limited under EC Directive on Drinking Water Quality 80/778/EEC. Phosphorus: guide level 400 µg l⁻¹; maximum admissible concentration 5000 µg l⁻¹ (as P₂O₅). Sodium: guide level 20 mg l⁻¹; maximum admissible concentration 150 mg l⁻¹ (3).

References

1. Smyth, H. F. et al *Am. Ind. Hyg. Assoc. J.* 1969, 30, 470.
2. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
3. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

T361 tritolyl phosphate



C₂₁H₂₁O₄P

Mol. Wt. 368.37

CAS Registry No. 1330-78-5

Synonyms phosphoric acid, tris(methylphenyl) ester; tricresyl phosphate; TCP (plasticiser); Celluflex; Lindol; PX-917

EINECS No. 215-548-8

RTECS No. TD 0175000

Uses Plasticiser, solvent and flame retardant.

Physical properties

B. Pt. ~265°C at 10 mmHg **Flash point** >110°C **Specific gravity** 1.16 at 25°C with respect to water at 25°C
Solubility Organic solvents: acetone, ethanol

Occupational exposure

Supply classification toxic, dangerous for the environment

Risk phrases Toxic: danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R39/23/24/25, R51/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – When using do not eat, drink or smoke – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S20/21, S28, S45, S61)

Ecotoxicity

Fish toxicity

Toxicity to a variety of fish species has been reviewed (1).

Environmental fate

Degradation studies

Degraded in river water by bacteria that appears to use the compound as a carbon source (species unspecified) (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 5.19 g kg⁻¹ (2).

LD_{Lo} oral rabbit 100 mg kg⁻¹ (3).

LD₅₀ dermal cat 1.5 g kg⁻¹ (4).

Carcinogenicity and chronic effects

The National Toxicology Program tested rats and mice via feed. No evidence for carcinogenicity in either species (5).

Teratogenicity and reproductive effects

Ovarian toxicity in mice seen during the NTP study included non-malignant hypoplasia, atrophy, follicular necrosis and tubular hyperplasia (5-7).

Swiss mice used in continuous breeding study revealed impaired fertility in both sexes. Mice received 0.05-0.2% of compound in diet. ♂ offspring also showed impaired fertility and reduced sperm motility (8).

Irritancy

Dermal rabbit (24 hr) 500 mg (non-occluded) and 500 mg instilled into rabbit eye for 24 hr caused mild irritation (9).

Other comments

Pollutant of land and river water (10).

Toxicity to a variety of fish species has been reviewed (11).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (12).

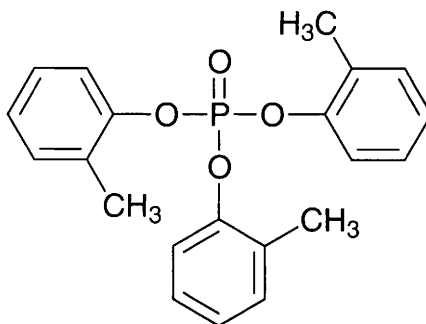
The substance is a mixture of isomeric tritolyl phosphates, usually excluding as much as possible the very toxic *ortho*-isomer.

References

1. Kawai, S. et al *Annu. Rep. Osaka City Inst. Public Health Environ. Sci.* 1985, **48**, 175-183.
2. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Propravku* 1972, Prague, Czechoslovakia.
3. Lefaux, R. *Practical Toxicology of Plastics* 1968, Chemical Rubber Co., Cleveland, OH, USA.
4. *Toxicol. Lett.* 1980, **1000**(sp 1), 14.
5. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-433, NIEHS, Research Triangle Park, NC, USA.

6. Maronpot, R. *EHP, Environ. Health Perspect.* 1987, **13**, 125-130.
7. Morrissey, R. E. et al *Fundam. Appl. Toxicol.* 1988, **11**(2), 359-371.
8. Chapin, R. E. *Fundam. Appl. Toxicol.* 1988, **10**(2), 344-354.
9. *Union Carbide Data Sheet* 29 Dec 1964.
10. Fukushima, M. et al *Annu. Rep. Osaka City Inst. Public Health Environ. Sci.* 19876, **49**, 11-20 (Japan.) (*Chem. Abstr.* **108**, 118532b).
11. van den Dikkenberg, R. P. et al *Gov. Rep. Announce Index (U. S.)* 1990, **90**(1c), Abstr. No. 048,945.
12. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

T362 tri-*o*-tolyl phosphate



C₂₁H₂₁O₄P

Mol. Wt. 368.37

CAS Registry No. 78-30-8

Synonyms phosphoric acid, tris(2-methylphenyl) ester; phosphoric acid, tri-*o*-tolyl ester; *o*-cresyl phosphate; tri-*o*-cresyl phosphate; tris(*o*-methylphenyl) phosphate

EINECS No. 201-103-5

RTECS No. TD 0350000

Uses Plasticiser.

Physical properties

M. Pt. 11°C **B. Pt.** 410°C **Specific gravity** 1.17 **Volatility** v.p. v. p. 10 mmHg at 265°C; v.den. 12.7

Solubility Organic solvents: diethyl ether, ethanol

Occupational exposure

FR-VME 0.1 mg m⁻³

UK-LTEL 0.1 mg m⁻³

US-TWA 0.1 mg m⁻³

UK-STEL 0.3 mg m⁻³

UN No. 2574 **HAZCHEM Code** 2X **Conveyance classification** toxic substance

Supply classification toxic, dangerous for the environment

Risk phrases Toxic: danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R39/23/24/25, R51/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – When using do not eat, drink or smoke – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S20/21, S28, S45, S61)

Ecotoxicity

Invertebrate toxicity

IC₅₀ (24 hr) *Ankistrodesmus falcatus* var. *acicularis*, *Scenedesmus quadricauda* 2.5, 4.2 mg l⁻¹, respectively, at 20°C (1).
LD₁₃ *Aedes aegypti* 0.1 mg l⁻¹ (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1160 mg kg⁻¹ (3).

LD₅₀ oral rat, rabbit 8400, 3700 mg kg⁻¹, respectively (4).

LD_{Lo} intraperitoneal rabbit 100 mg kg⁻¹ (5).

LD_{Lo} intravenous rabbit 100 mg kg⁻¹ (5).

LD_{Lo} subcutaneous rabbit, dog 100 mg kg⁻¹ (5).

LD_{Lo} subcutaneous cat 185 mg kg⁻¹ (6).

Oral sheep single dose of 100, 200 or 400 mg kg⁻¹. Animals exhibited acute intoxication characterised by diarrhoea, dehydration, metabolic acidosis and death within 6 days (7).

Oral pig single dose of 100-1600 mg kg⁻¹. Animals showed minimal signs of acute intoxication but developed severe signs of delayed neuropathy ~15 days after receiving the dose (7).

Teratogenicity and reproductive effects

Oral rat (days 6-18 gestation) 87.5, 175 and 350 mg kg⁻¹ day⁻¹. At 87.5 and 175 mg kg⁻¹ no maternal toxicity or deaths were observed; maternal deaths at 350 mg kg⁻¹ were higher than those in the control group. No significant differences were seen in the frequency of malformations between treated and control rats (8).

Oral ♂ rat (63 days) 10-100 mg kg⁻¹ day⁻¹. The threshold dose for observable testicular toxicity was 10-25 mg kg⁻¹ day⁻¹. At ≥25 mg kg⁻¹ day⁻¹ testicular pathological changes were seen, including PAS-positive droplets, immature germ cells and multinucleate giant cells in the lumen. The compound interfered directly with spermatogenic processes and sperm motility and not via androgenic mechanisms or decreased vitamin E availability (9).

In mice tri-*o*-cresyl phosphate caused an increase in maternal mortality and a decreased number of viable litters, but had no effect on litter size or birth weight gain when administered at 10 ml kg⁻¹ day⁻¹ (duration unspecified) (10).

Metabolism and toxicokinetics

Following a single dermal dose to cats the highest concentration of the compound was found in plasma after 12 hr and metabolites were at their highest concentration between 24-48 hr. The parent compound was the predominant compound in the brain, spinal cord and sciatic nerve, while the metabolites *o*-hydroxybenzoic acid and di-*o*-cresyl phosphate were predominant in the liver, kidney and lung (11).

Dermal absorption in humans is ~100 × faster than in dogs; significant dermal absorption appears to occur in cats (12).

Metabolism occurs via three pathways. The first involves hydroxylation of one or more of the methyl groups forming hydroxymethyl compounds and *o*-hydroxybenzyl alcohol (saligenin). The hydroxymethyl is cyclised to form saligenin cyclic *o*-tolyl phosphate, the neurotoxic metabolite. The second pathway is dearylation of the *o*-cresyl groups and the third involves further oxidation of the hydroxymethyl to aldehyde and carboxylic acid (12). Excretion is mainly via the urine and faeces with small amounts eliminated in expired air (12).

Hens were given a single oral dose of the ¹⁴C-labelled compound. Highest concentrations in plasma were found 0.5-1 day after administration; t_{1/2} was 2 days. Saligenin cyclic *o*-tolyl phosphate had t_{1/2} of 2.06, 1.36, 1.11 and 4.44 days in plasma, liver, kidneys and lungs, respectively (13).

Other effects

Other adverse effects (human)

The initial symptoms of poisoning include nausea, vomiting, abdominal pain and diarrhoea, and may last from a few hr to a few days. Longer-term symptoms, which are usually delayed by 3-28 days, are neurological and often lead to paralysis and pyramidal signs (spasticity, etc.). If small cumulative doses are taken the initial symptoms may not be present. There is also considerable variation in the sensitivity of individuals to the compound; 0.15 g caused severe symptoms in one subject while others were unaffected by 1-2 g (12).

Any other adverse effects

Gavage ♂ rat (63 day) 10-100 mg kg⁻¹ day⁻¹. Animals showed no consistent neurobehavioural alterations associated with organophosphorus-induced delayed neurotoxicity. Gavage chickens (18 days) 100 mg kg⁻¹ day⁻¹. Birds developed delayed neurotoxicity characterised by ataxia which progressed to paralysis (14).

Other comments

The active metabolite of the compound, saligenin cyclic *o*-tolyl phosphate, caused decreased germination of kidney beans and wheat (15).

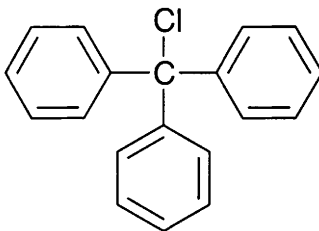
Reviews on human health effects, experimental toxicology, workplace experience, environmental effects, ecotoxicology, exposure levels listed (16).

Human poisoning reviewed (17).

References

1. Wong, P. T. S. et al *Sci. Total Environ.* 1984, **32**(2), 157-165.
2. Quinstad, G. B. et al *Pestic. Biochem. Physiol.* 1975, **5**, 233-241.
3. Veronesi, B. et al *Toxicologist* 1984, **4**, 55.
4. Johannsen, F. R. et al *Toxicol. Appl. Pharmacol.* 1977, **41**, 291-304.
5. *Arch. Exp. Pathol. Pharmacol.* 1932, **168**, 473.
6. *Bull. Johns Hopkins Hospital* 1933, **52**, 39.
7. Wilson, R. D. et al *Am. J. Vet. Res.* 1982, **43**(11), 1954-1957.
8. Tocco, D. R. et al *Fundam. Appl. Toxicol.* 1987, **8**(3), 291-297.
9. Somkuti, S. C. et al *Toxicol. Appl. Pharmacol.* 1987, **89**, 49-63.
10. Report 1987, Order No. PB89-139075, Environmental Health Research and Testing Inc., Cincinnati, OH, USA.
11. Nomeir, A. A. et al *Drug Metab. Disp.* 1984, **12**(6), 705-711.
12. *IPCS Environmental Health Criteria No. 110: Tricresyl Phosphate* 1990, WHO, Geneva, Switzerland.
13. Suwita, E. et al *Arch. Toxicol.* 1990, **64**(3), 237-241.
14. Somkuti, S. G. et al *Fundam. Appl. Toxicol.* 1988, **10**(2), 199-205.
15. Eto, M. et al *Biochem. Pharmacol.* 1962, **11**, 337-352.
16. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
17. Inoue, N. et al *Sangyo-Ika-Daigaku-Zasshi* 1988, **10**(4), 433-442.

T363 trityl chloride



C₁₉H₁₅Cl

Mol. Wt. 278.78

CAS Registry No. 76-83-5

Synonyms 1,1',1''-(chloromethyldiyl)trisbenzene; chlorotriphenylmethane; triphenylmethyl chloride

EINECS No. 200-986-4

RTECS No. PA 6450000

Physical properties

M. Pt. 110-112°C B. Pt. 230-235°C at 20 mmHg

Mammalian & avian toxicity

Acute data

LD₅₀ intravenous mouse 180 mg kg⁻¹ (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine: guide level 1 µg l⁻¹,

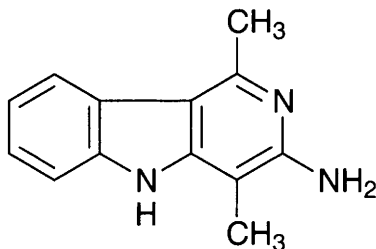
Phenols: maximum admissible concentration 0.5 µg l⁻¹ (2).

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (3).

References

1. Report NX 04021, US Army Armament Research and Development Command, Chemical Systems Laboratories, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD, USA.
2. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
3. S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations 1991, HMSO, London, UK

T364 Trp-P-1



C₁₃H₁₃N₃

Mol. Wt. 211.27

CAS Registry No. 62450-06-0

Synonyms 3-amino-1,4-dimethyl-γ-carboline; 3-amino-1,4-dimethyl-5H-pyrido[4,3-b]indole; tryptophan-P-1

RTECS No. UU 9351900

Occurrence Pyrolysis product of cooked food, especially sardines.

Physical properties

M. Pt. 252-260°C

Solubility Organic solvents: methanol

Environmental fate

Abiotic removal

After a 30 min irradiation by a mercury vapour lamp, mutagenic activity was reduced to less than half (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, hamster 200, 380 mg kg⁻¹, respectively (2).

Carcinogenicity and chronic effects

No adequate data for evidence of carcinogenicity to humans, sufficient evidence for carcinogenicity in animals, IARC classification group 2B (3,4).

Subcutaneous neonatal mice, observed for 1 yr, induced liver tumours in 45% of ♂ and malignant lymphomas in 13% of ♂ and in 24% of ♀ (5).

ICR mice (1 yr) 50 µg g⁻¹ induced lung, liver, lymphoma tumours and leukaemia in both ♂ and ♀ animals (6).

Hepatocellular carcinomas reported in rats and mice given 0.02-0.08% in the diet (7,8).

Genotoxicity

Salmonella typhimurium TA98, TA100 with metabolic activation positive (8).

Salmonella typhimurium NM2009 with metabolic activation positive (9).

Escherichia coli K12, PG37 and PQ35 SOS Chromotest with metabolic activation positive (10).

Induced sister chromatid exchanges in cultured human lymphocytes with metabolic activation (11).

Drosophila melanogaster DNA-repair test positive (12).

Intraperitoneal *in vivo* rat bone marrow cells (5 daily injections) 0.210-10.5 ng kg⁻¹ dose-response relationship obtained (13).

Caused cytotoxicity in the form of the leakage of DNase and death of cells in rat hepatocytes (14).

Other effects

Any other adverse effects

Taken up into PC12h cells by the transport system specific for dopamine, accumulated in cells and reduced the enzyme activity of tyrosine hydroxylase and aromatic L-amino acid decarboxylase (15).

Other comments

The geometric mean value of the concentrations of Trp-P-1 found at 11 locations in the Yodo River systems (Japan) was 26.9 ng g⁻¹ blue rayon equivalent (16).

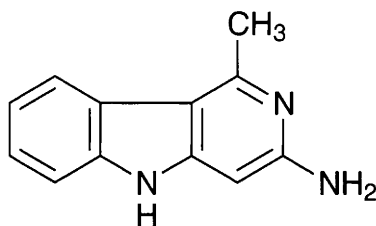
Human health effects and experimental toxicology reviewed (3).

Identified in human, cataractous lenses, but not in young bovine lenses, concentrated in the insoluble lens proteins (17).

References

1. Yoo, Y. S. et al *Environ. Mutagen. Carcinog.* 1989, 8(2), 99-104.
2. Miller, E. C. et al (Ed.) *Naturally Occurring Carcinogens – Mutagens and Modulators of Carcinogenesis* 1979, 167, Japan. Sec. Soc., Tokyo, Japan.
3. *IARC Monograph* 1983, 31, 247.
4. *IARC Monograph* 1987, **Suppl.** 7, 73.
5. Fujii, K. et al *Carcinogenesis (London)* 1987, 8(11), 1721-1723.
6. Fujii, K. *Carcinogenesis (London)* 1991, 12(8), 1409-1415.
7. Ohyaki, H. et al *Environ. Health Perspect.* 1986, 67, 129-134.
8. Takayama, S. et al *Jpn. J. Cancer Res.* 1985, 76(9), 815-817.
9. Oda, Y. et al *Mutat. Res.* 1995, 334(2), 145-156.
10. Thybaud-Lambay, V. et al *Mutat. Res.* 1986, 173(3), 177-180.
11. Inoue, K. et al *Mutat. Res.* 1983, 117(3-4), 301-309.
12. Obana, H. et al *Jpn. J. Toxicol. Environ. Health* 1993, 39(6), 577-581.
13. Fujii, K. et al *Kobe Daigaku Igakubu Kiyo* 1987, 48(4), 247-252 (Jap.) (*Chem. Abstr.* 109, 793e).
14. Segawa, T. et al *Chemosphere* 1994, 28(5), 853-861.
15. Takahasi, T. et al *Adv. Behav. Biol.* 1990, 38A, 345-348.
16. Ohe, T. *Mutat. Res.* 1997, 393(1,2), 73-79.
17. Manabe, S. et al *Exp. Eye Res.* 1989, 48(3), 351-363

T365 Trp-P-2



$C_{12}H_{11}N_3$

Mol. Wt. 197.24

CAS Registry No. 62450-07-1

Synonyms 3-amino-1-methyl-5H-pyrido[4,3-b]indole; 3-amino-1-methyl- γ -carboline; 1-methyl-5H-pyrido[4,3-b]indol-3-amine; tryptophan P2

RTECS No. UU 9354000

Occurrence Broiled fish and meat.

Physical properties

M. Pt. 248-250°C

Solubility Organic solvents: methanol

Mammalian & avian toxicity

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2B (1).

ICR mice (1 yr) 25 $\mu\text{g g}^{-1}$ induced tumours of lung and liver in σ mice and tumours of the lymphatic system or leukaemia in φ mice (2).

Dermal application of 2 $\text{mg } 2 \times \text{wk}^{-1}$ for 5 wk to φ mice followed by 2.5 μg TPA (CAS RN. 16561-29-8) caused skin squamous cell papillomas and carcinomas. Alone it did not cause skin tumours, indicating it acts mainly as an initiator rather than a complete carcinogen (3).

Genotoxicity

Salmonella typhimurium TA98 with metabolic activation positive (4).

Salmonella typhimurium TA98, TA100 with metabolic activation positive (5).

Escherichia coli K12, PG37 and PQ35 SOS Chromotest with metabolic activation positive (4,6).

Drosophila melanogaster (white/white⁺) eye mosaic assay interchromosomal mitotic recombination positive (7).

Drosophila melanogaster DNA-repair test positive (8).

Caused DNA single-strand breaks and cell injury in rat hepatocytes (9).

Chinese hamster lung fibroblasts induced diptheria toxin resistant mutations (10).

Intraperitoneal administration of 4.2 $\text{mg kg}^{-1} \text{ day}^{-1}$ to mice on day 8-9 pregnancy; mammalian mutagenicity spot test positive (11).

Other comments

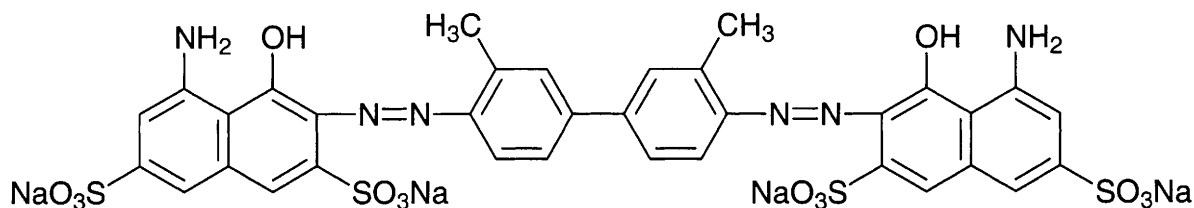
The geometric mean value of the concentrations of Trp-P-2 found at 11 locations in the Yodo River systems (Japan) was 37.3 ng g^{-1} blue rayon equivalent (12).

Human health effects and experimental toxicology reviewed (13).

References

1. IARC Monograph 1987, **Suppl. 7**, 73.
2. Fujii, K. *Carcinogenesis (London)* 1991, **12**(8), 1409-1415.
3. Takahashi, M. et al *Jpn. J. Cancer Res.* 1986, **77**(6), 509-513.
4. Mersch-Sundermann, V. et al *Mutagenesis* 1994, **9**(3), 205-224.
5. Nagao, M. et al *Carcinogenesis (London)* 1980, **1**, 451.
6. Thybaud-Lambay, V. et al *Mutat. Res.* 1986, **173**(3), 177-180.
7. Vogel, E. W. et al *Mutagenesis* 1993, **8**(1), 57-81.
8. Obana, H. et al *Jpn. J. Toxicol. Environ. Health* 1993, **39**(6), 577-581.
9. Segawa, T. et al *Chemosphere* 1993, **27**(4), 565-576.
10. Tenada, M. et al (Ed.) *International Conference on Environmental Mutagens* 1981, Tokyo, Japan.
11. Jensen, N. J. *Cancer Lett.* 1983, **20**(2), 241-244.
12. Ohe, T. et al *Mutat. Res.* 1997, **393**(1,2), 73-79.
13. IARC Monograph 1983, **31**, 255

T366 Trypan Blue



$C_{34}H_{24}N_6Na_4O_{14}S_4$

Mol. Wt. 960.82

CAS Registry No. 72-57-1

Synonyms 3,3'-[(3,3'-dimethyl(1,1'-biphenyl)-4,4'-diyl)]bis(azo)]bis(5-amino-4-hydroxy)-2,7-naphthalenedisulfonic acid, tetrasodium salt; C.I. Direct Blue 14; 3,3'-[(3,3'-dimethyl-4,4'-biphenylene)bis(azo)]bis(5-amino-4-hydroxy-2,7-naphthalenedisulfonic acid) tetrasodium salt; sodium ditolyldiazobis-8-amino-1-naphthol-3,6-disulfonate; Benzamine Blue; Congo Blue

EINECS No. 200-786-7

RTECS No. QJ 6475000

Uses Biological stain and dye for textiles leather and paper. Therapeutic agent for sleeping sickness and topically for some viral infections.

Physical properties

M. Pt. >300°C

Solubility Water: 20 g l⁻¹. Organic solvents: cellosolve

Environmental fate

Degradation studies

In an aqueous biodegradation screening test (7 day) with anaerobic sludge inoculums >90% degradation was observed, 4,4'-diamino-3,3'-dimethylbiphenyl was identified as a metabolite (1).

Can be degraded anaerobically by microorganisms to amines which can be further degraded aerobically (species unspecified) (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 6.2 g kg⁻¹ (2).

LD_{Lo} intraperitoneal rat, mouse 300-350 mg kg⁻¹, respectively (3).

LD_{Lo} intravenous rat 300 mg kg⁻¹ (3).

LD_{Lo} intraperitoneal rabbit 400 mg kg⁻¹ (3).

LD_{Lo} subcutaneous guinea pig 300 mg kg⁻¹ (3).

Sub-acute and sub-chronic data

When injected into rats 200-400 mg kg⁻¹ at 2 wkly intervals subcutaneously (duration unspecified), anaemia with leucopenia and thrombocytopenia has been produced (4).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2B (5).

No tumours were reported in studies in which rats received the compound orally for ≤1 yr (6,7).

Tumours of the reticulo-endothelial system have been seen in rats receiving the substance subcutaneously in a number of studies (8-10).

Intraperitoneal injection has also resulted in tumours (species unspecified) (11,12).

Mice receiving the substance subcutaneously have been reported not to produce tumours (13,14).

Teratogenicity and reproductive effects

Pregnant rats receiving 20-120 mg kg⁻¹ intraperitoneally as a 1% solution on day 8 yielded fetuses which had skeletal and visceral malformations at day 20. ♂ fetuses were more sensitive than ♀, and Wistar-Mishima rat were more sensitive than BDIX rats (15).

Metabolism and toxicokinetics

After subcutaneous or intraperitoneal injection, the compound is rapidly absorbed and distributed throughout the body. Maximum serum concentrations are reached within 2 hr with binding to plasma proteins (16,17).

Exponential decline of plasma levels occurs due to rapid excretion and uptake by the reticulo-endothelial system (16-18).

In vitro rat liver can reduce the compound to *o*-toluidine and 2,8-diamino-1-naphthol-3,6-disulphonic acid (19).

Genotoxicity

Salmonella typhimurium TA1538 with metabolic activation weakly positive; after dithionite reduction TA98, TA1538 positive (20).

Escherichia coli PQ36 SOS chromotest negative (21).

In vitro rat and hamster hepatocytes yielded positive results in a DNA repair assay (22).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (23).

The toxicology of the compound has been reviewed (24).

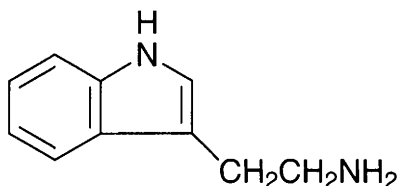
The substance is difficult to purify, thus some biological effects described as being caused by Trypan Blue may have been produced by impurities (24).

References

1. Brown, D. et al *Chemosphere* 1987, **16**(7), 1539-1553.
2. *Office of Toxic Substances Report 215154* US EPA, Office of Toxic Substances, 401 M. St., Washington, DC, USA.
3. *Proc. Soc. Exp. Biol. Med.* 1934, **31**, 825.
4. Brown, D. V. et al *Blood* 1961, **18**, 543-560.
5. *IARC Monograph* 1987, **Suppl. 7**, 73.
6. Oka, K. et al *Gann* 1957, **48**, 573-575.
7. Ooneda, G. *Gunma J. Mol. Sci.* 1957, **6**, 295-317.
8. Gillman, T. et al *Cancer* 1952, **5**, 792-846.

9. Gillman, T. et al *J. Natl. Cancer Inst.* 1973, **50**, 1179-1193.
10. Brown, D. V. et al *Proc. Soc. Exp. Biol. (N.Y.)* 1963, **114**, 290-293.
11. Papacharalampous, N. X. *Beitr. Path. Anal.* 1957, **117**, 85-89.
12. Papacharalampous, N. X. *Frankfurt Z. Path.* 1966, **75**, 74-77.
13. Tomatis, L. *Acta Un. Inst. Cancer* 1963, **19**, 607-611.
14. Tomatis, L. *Tumori*, 1966, **52**, 1-16.
15. Hoshino, K. et al *Teratology* 1988, **37**(1), 43-50.
16. Dijkstra, J. et al *S. Afr. J. Med. Sci.* 1960, **25**, 119-131.
17. Belitskii, G. A. *Bull. Exp. Biol. Med.* 1963, **55**, 523-525.
18. Thilander, H. *Acta Path. Microbiol. Scand.* 1963, **57**, 57-59.
19. Lloyd, J. B. et al *The interaction of drugs and subcellular components in animal cells* Campbell, P. N. (Ed.), Jr A Churchill, London, UK.
20. Joachim, F. et al *Mut. Res.* 1985, **156**, 131-138.
21. Von der Hude, W. *Mutat. Res.* 1988, **203**(2), 81-94.
22. Barfknecht, T. R. et al *Cell Biol. Toxicol.* 1987, **3**(2), 193-207.
23. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium.
24. *IARC Monograph* 1975, **8**, 267

T367 tryptamine



$C_{10}H_{12}N_2$

Mol. Wt. 160.22

CAS Registry No. 61-54-1

Synonyms 1H-indole-3-ethanamine; 3-(2-aminoethyl)indole; 2-(3-indolyl)ethylaniline

EINECS No. 200-510-5

RTECS No. NL 4020000

Occurrence Occurs in plants. Can be found in human urine and blood.

Physical properties

M. Pt. 118°C **B. Pt.** 137°C at 0.15 mmHg

Solubility Organic solvents: acetone, ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat 223 mg kg⁻¹ (1).

LD₅₀ intraperitoneal mouse 100 mg kg⁻¹ (2).

LD₅₀ subcutaneous mouse 500 mg kg⁻¹ (3).

Sub-acute and sub-chronic data

Intravenous doses of 25 mg kg⁻¹ to mice induce the 5-HT syndrome of head weaving and hind limb abduction. This has been attributed to the binding of tryptamine to 5-HT₂ receptors and subsequent agonistic actions (4,5).

Other comments

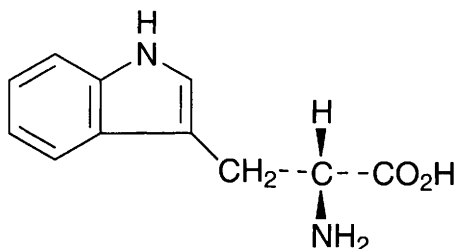
The presence in human urine on some occasions may be explained by being a product of bacterial metabolism in the large intestine (6).

Neural binding sites can be detected in mammalian and human brain (4,5,7).

References

1. *J. Pharm. Sci* 1977, **66**, 1692.
2. *Eur. J. Med. Chem.* 1974, **9**, 453.
3. *Diss. Pharm. Pharmacol.* 1970, **22**, 313.
4. Sagimoto, Y. et al *Neuropharmacology* 1986, **25**(11), 1289-1291.
5. Yamada, J. et al *Eur. J. Pharmacol.* 1987, **140**, 323-330.
6. Perry, et al *Clin. Chim. Acta* 1966, **14**, 1161.
7. Korneev, A. Ya *Byull Eksp. Biol. Med.* 1988, **105**(1), 41-43 (Russ.) (*Chem. Abstr.* **109**, 733k)

T368 D-tryptophan



$C_{11}H_{12}N_2O_2$

Mol. Wt. 204.23

CAS Registry No. 153-94-6

EINECS No. 205-819-9

RTECS No. YN 6129000

Uses Used with L-tryptophan in dietary supplements.

Physical properties

M. Pt. 282-285°C (decomp.)

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat 4289 mg kg⁻¹ (1).

Metabolism and toxicokinetics

The compound is well absorbed from the mammalian gastro-intestinal tract, and *in situ* disappearance studies using rats, absorption is similar to that of L-tryptophan (2).

It is distributed to most tissues including the central nervous system (2-4) and has been shown capable of crossing the human placental barrier (4).

When administered to rats it can increase brain levels of 5-HT and its metabolites (3).

In the wall of the rabbit small intestine it binds to the haemoprotein indoleamine 2,3-dioxygenase, but can also bind to other proteins such as albumin (5).

Genotoxicity

Salmonella typhimurium TA92, TA94, TA98, TA100, TA1535, TA1537 with metabolic activation negative (6).

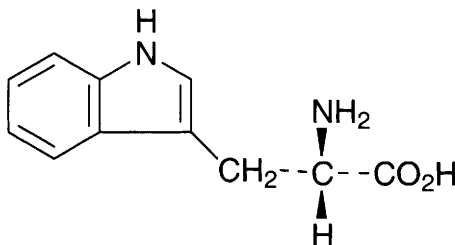
In vitro chromosome aberration in Chinese hamster fibroblasts CHL without metabolic activation negative (6).

Chinese hamster V79 cell metabolic cooperation assay positive (7).

References

1. Arch. Biochem. Biophys. 1956, **64**, 319.
2. Mizuno, M. et al Toxicol. Appl. Pharmacol. 1989, **9**(3), 415-425.
3. Aliev, M. G. Izv. Akad. Nauk. SSR Ser. Biol. Nauk. 1987(2), 94-100 (Russ.) (Chem. Abstr. **10**, 1915x).
4. Johnson, L. W. et al Am. J. Physiol. 1988, **254** (6, pt 1), C773-C780.
5. Sono, M. Biochemistry 1990, **29**(6), 1451-1460.
6. Ishidate, M. Fed. Chem. Toxicol. 1984, **22**(8), 623-636.
7. Bohrman, J. S. et al Environ. Mol. Mutagen. 1988, **12**(1), 33-51

T369 L-tryptophan



C₁₁H₁₂N₂O₂

Mol. Wt. 204.23

CAS Registry No. 73-22-3

Synonyms α-amino-β-(3-indolyl)propionic acid; 1-β-3-indolylalanine; 2-amino-3-indolylpropanoic acid; L-Trp; Optimax; Neurocalm

EINECS No. 200-795-6

RTECS No. YN 6130000

Uses Anti-depressant, nutrient.

Occurrence An essential amino acid present in plants and animals.

Physical properties

M. Pt. 289°C (decomp.)

Solubility Water: 11.4 g l⁻¹ at 25°C. Organic solvents: hot ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat 1.63 g kg⁻¹ (1).

LD₅₀ intraperitoneal mouse 4.8 g kg⁻¹ (2).

Carcinogenicity and chronic effects

National Toxicology Programme tested rats and mice via feed. No evidence of carcinogenicity was seen in either species of either sex (3).

Subcutaneous rat (2 yr) 20 mg wk⁻¹. Malignant tumours in the uterus, mammary gland fibroadenomas, salivary gland adenomas, mesenteric reticulosarcomas and reticuloleukosis were observed (4).

Metabolism and toxicokinetics

L-Tryptophan is well absorbed from the mammalian small intestine (5,6) and to some extent from the stomach (7). Distributed throughout the body, but incompletely metabolised by most animals. Products of incomplete oxidation appear in urine and include indole-3-acetic acid and anthranilic acid (8).

Precursor of the neurotransmitter 5-HT, which is formed by oxidation of L-tryptophan to 5-hydroxytryptophan followed by decarboxylation, both occurring in neural tissue (9-12).

Circulation L-tryptophan levels can influence the synthesis of 5-HT and this is the basis of the use of L-tryptophan as an anti-depressant agent (10-13).

Extensively bound to plasma albumin (14,15).

Genotoxicity

Salmonella typhimurium TA92, TA94, TA98, TA100, TA1535, TA1537 with metabolic activation negative (16).

In vitro chromosome aberration in Chinese hamster fibroblasts CHL without metabolic activation negative (16).

In vitro human lymphocyte cells DNA synthesis inhibition positive (17).

In vitro rat liver hepatocyte cells DNA synthesis inhibition positive (18).

Other effects

Other adverse effects (human)

Nausea, headache, lightheadedness and drowsiness have been reported as side effects. Tryptophan-containing products have been associated with the eosinophilia-myalgia syndrome, but contamination of tryptophan during the manufacturing process may have been responsible (15).

From late 1989, reports arose of patients developing the syndrome over several wk, even if they had previously taken the compound without untoward effect. Evidence pointed to contamination coming from a single manufacturer and taking the form of bacitracin-like peptides (19-22).

Other comments

Reduces sister chromatid exchange incidence in rats treated with cyclophosphamide (23).

The pharmacokinetics following oral and intravenous administration have been reviewed (14).

The probability of mutagenic derivatives being formed from tryptophan during certain food preparation procedures has been assessed (24).

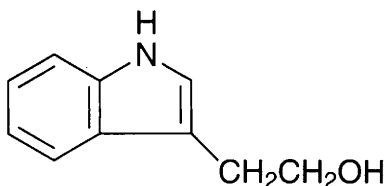
A 1% solution in water has a pH of 5.5 to 7 (15).

References

1. Arch. Biochem. Biophys. 1955, **58**, 253.
2. Iyakuhi Kenkyu 1980, **11**, 635.
3. National Toxicology Program Research and Testing Division 1992, Report No. TR-071, Research Triangle Park, NC, USA.
4. Dzhioev, F. K. Vopr. Onkol. 1974, **20**(8), 75-81.
5. Mizuno, M. et al Toxicol. Appl. Pharmacol. 1989, **97**(3), 415-425.
6. Rerat, A. et al Nutr. Rep. Int. 1988, **37**(1), 179-188.
7. Bravo, I. R. Med. Sci. Res. 1989, **17**(12), 523-524.
8. Jacoby, et al Biochem. Biophys. Res. Commun. 1962, **8**, 357.
9. Jequier, et al Mol. Pharmacol. 1967, **3**, 274.
10. Huether, G. Neurochem. Res. 1986, **11**(12), 1663-1668.
11. Young, S. N. Prog. Neuro-Psychopharmacol. Biol. Psychiatry 1989, **13**(3-4), 373-379.
12. Dikio, M. et al J. Neurochem. 1991, **56**(1), 153-162.
13. Barker, W.A. Int. Clin. Psychopharmacol. 1987, **2**, 261-272.
14. Green, A. R. et al Br. J. Clin. Pharmacol. 1985, **20**, 317-321.
15. Martindale: The Extra Pharmacopoeia 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
16. Ishidate, M. Food Chem. Toxicol. 1984, **22**(8), 623-636.
17. Novogradsky, A. et al Proc. Natl. Acad. Sci. USA 1982, **79**(4), 1171-1174.
18. Novicki, D. L. et al Cancer Res. 1985, **45**(1), 337-344.
19. Slutsker, L. et al J. Am. Med. Assoc. 1990, **264**, 213-217.

20. Belongia, E. A. et al *New Engl. J. Med.* 1990, **323**, 357-365.
21. Varga, J. et al *Ann. Intern. Med.* 1992, **116**, 140-147.
22. Barnhart, E. R. et al *Lancet* 1990, **336**, 695-696.
23. Chen, J. F. *Cytologia* 1987, **52**(3), 687-692.
24. Overvik, E. et al *Carcinogenesis (London)* 1989, **10**(12), 2293-2301

T370 tryptophol



$C_{10}H_{11}NO$

Mol. Wt. 161.20

CAS Registry No. 526-55-6

Synonyms 2-(3-indolyl)ethyl alcohol; 1*H*-indole-3-ethanol; 3-indolyethanol; indole ethanol; 3- β -hydroxyethylindole

EINECS No. 208-393-2

RTECS No. KL 3685000

Occurrence Metabolite in many microorganisms. In young wines (1).

Physical properties

M. Pt. 59°C B. Pt. 174°C at 20 mmHg

Solubility Water: slightly soluble. Organic solvents: ethanol, methanol

Environmental fate

Degradation studies

Accelerated anaerobic treatment of wastewater from wine production can result in 99.9% degradation of the compound (2).

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal mouse 351 mg kg⁻¹ (3).

LD₅₀ intravenous mouse 180 mg kg⁻¹ (4).

Other comments

The antioxidant activity, anticarcinogen and hepatoprotectant properties of the compound have been reviewed (5).

References

1. Gil, C. et al *Food Chem.* 1986, **22**(1), 59-65.
2. Crespo, R. *Comm. Eur. Communities [Rep.]* EUR1988, EUR11350, 323-328.
3. *J. Toxicol. Env. Health* 1976, **1**, 515.
4. NIOSH NX No. 00777, U. S. Army Armament Research & Development Command, Chemical Systems Laboratory, NIOSH Exchange Chemicals, Aberdeen Proving Ground, MD, USA.
5. Tabor, M. et al *Adv. Exp. Med. Bio.* 1991, **283**, 833-836

T371 tungsten

W

W

Mol. Wt. 183.85

CAS Registry No. 7440-33-7

EINECS No. 231-143-9

RTECS No. YO 7175000

Uses To harden tips of tools, in plating and in x-ray apparatus.

Occurrence Occurs as tungstates in wolframite and scheelite and in traces in seawater. Comprises ~1.5 ppm of the earth's crust.

Physical properties

M. Pt. 3410°C B. Pt. 5927°C Specific gravity 19.3 at 20°C

Occupational exposure

SE-LEVL 5 mg m⁻³

UK-LTEL 5 mg m⁻³

US-TWA 5 mg m⁻³

UK-STEL 10 mg m⁻³

US-STEL 10 mg m⁻³

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat 5 g kg⁻¹ (1).

Intrathecal inoculation into laboratory animals causes pigmentation and interstitial cell proliferation near particles. Bronchiolitis can result (form unspecified) (2).

Carcinogenicity and chronic effects

When administered to ♀ rats at 150 ppm in diet for 15 days, the element had a promoting effect with respect to mammary carcinogenesis induced by methylnitrosourea (form unspecified) (3).

Metabolism and toxicokinetics

The element in metallic form is not well absorbed from the mammalian gastro-intestinal tract (1).

When administered to rats in drinking water for 6 months, the element influenced tissue and bone distribution of Cu, Ni, Pb and Mo (form unspecified) (4).

When fed in diet to mice, there was a loss of xanthine oxidase in the small intestine as judged by immunological and biochemical methods (form unspecified) (5).

Tungsten does not bind appreciably to proteins (6).

Irritancy

Dermal rabbit (24 hr) 500 mg caused mild irritation, as did the same dose applied to rabbit eye (form unspecified) (7).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (8).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (9).

The solubility and tissue handling of tungsten has been reviewed (6).

The element has been included in a study relating toxicity to results in *Salmonella typhimurium* mutagenicity tests (10).

References

1. Venugopal, B. et al *Metal Toxicity in Mammals* 2 1978, Plenum Press, New York, NY, USA.
2. Schepers, G. N. *Arch. Ind. Health* 1955, **12**, 134-136.
3. Wei, H. et al *Zhonghua Zhongliu Zazhi* 1987, **9**(3), 204-207 (Ch.) (*Chem. Abstr.* **108**, 1995p).
4. Nadeenko, V. G. et al *Gig. Sanit.* 1990, (6), 24-26 (Russ.) (*Chem. Abstr.* **113**, 92997h).
5. Manchester, K. M. *Intl. J. Biochem.* 1988, **20**(10), 1061-1066.
6. Edell, J. et al *Sci. Total Environ.* 1990, **95**, 107-117.
7. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
8. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
9. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
10. D'yachenko, Z. et al *Gig. Sanit.* 1990, (8), 83-85 (Russ.) (*Chem Abstr.* **113**, 186421t)

T372 tungsten carbide

CW

CW

Mol. Wt. 195.86

CAS Registry No. 12070-12-1

EINECS No. 235-123-0

RTECS No. YO 7250000

Uses Provides hard coatings for tools and ceramics.

Occupational exposure

SE-LEVL 5 mg m⁻³ (as W)

UK-LTEL 5 mg m⁻³ (as W)

US-TWA 5 mg m⁻³ (as W)

UK-STEL 10 mg m⁻³ (as W)

US-STEL 10 mg m⁻³ (as W)

Mammalian & avian toxicity

Carcinogenicity and chronic effects

The compound has been approved for study by the National Toxicology Program (1).

Irritancy

Dermal rabbit (24 hr) 500 mg caused mild irritation, as did the same dose applied to rabbit eye.

Other effects

Other adverse effects (human)

Adults working with tungsten carbide who were found to suffer from "hard metal" disease demonstrated difficulties in attention and verbal memory, along with abnormal visual and spatial memory (2).

Any other adverse effects

The compound had no effect *in vitro* on cell viability of mouse peritoneal cells or rat alveolar macrophages, but did potentiate the toxicity of cobalt dust (3).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (4).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (5).

References

1. *National Toxicology Program Research and Testing Division* 1992, NIEHS, Research Triangle Park, NC, USA.
2. Jordan, C. et al *Toxicol. Lett.* 1990, **54**(2-3), 241-243.
3. Lison, D. et al *Environ. Res.* 1990, **52**(2), 187-198.
4. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
5. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T373 tungsten hexafluoride



F₆W

Mol. Wt. 297.84

CAS Registry No. 7783-82-6

Synonyms tungsten fluoride

EINECS No. 232-029-1

RTECS No. YO 7720000

Uses Chemical intermediate.

Physical properties

M. Pt. 2.3°C B. Pt. 17.5°C Specific gravity 3.441 (liquid) at 15°C

Occupational exposure

DE-MAK 2.5 mg m⁻³ (as F) (total dust)

SE-LEVL 2 mg m⁻³ (as F)

UK-LTEL 2.5 mg m⁻³ (as F)

US-TWA 2.5 mg m⁻³ (as F)

UN No. 2196 Conveyance classification toxic gas, corrosive

Environmental fate

Abiotic removal

The compound can be removed from waste gases by dry scrubbing with dehydrated soda ash (1) or by cooling to <0°C followed by adsorption to remove the fluoride (2).

Mammalian & avian toxicity

Acute data

Rats exposed to 110 mg m⁻³ for 2 hr suffered toxic effects from fluoride that were prevented by pretreatment with repeated doses of glutamic acid, but not by a single dose of glutamic acid (3).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Fluoride: maximum admissible concentration 700 µg l⁻¹ at 25-30°C, 1500 µg l⁻¹ at 8-12°C (4).

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (5).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (6).

References

1. Yagi, T. et al *Jpn. Kokai Tokkyo Koho* JP 62, 152,519 [87,152,519] Appl. 85/297,598, 26 Dec 1985.
2. Fukushima, M. et al *Jpn. Kokai Tokkyo Koho* JP 62,273,038 [87,273,038] Appl. 86/116712, 21 May 1986.
3. Shugaev, V. A. *Gig. Tr. Prof. Zabol.* 1983, (12), 26-29 (Russ.) (*Chem. Abstr.* 100, 169476d).
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
5. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
6. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

T374 turpentine oil

CAS Registry No. 8006-64-2

Synonyms essential oils, turpentine; gum turpentine oil; oil of turpentine; spirits of turpentine; turpentine spirit

EINECS No. 232-350-7

RTECS No. YO 8400000

Uses As a constituent of ointments, wax and paint solvents, in polishes and related products. It can be used as an insecticide and in veterinary therapeutics.

Occurrence Turpentine oil is obtained by distillation and rectification of the oleo resin turpentine obtained from various species of pine and eucalyptus trees.

Physical properties

B. Pt. 154-170°C **Flash point** 35°C **Specific gravity** 0.854-0.868 at 25°C with respect to water at 25°C

Volatility v.den. 4.84

Solubility Organic solvents: chloroform, diethyl ether, ethanol

Occupational exposure

DE-MAK 100 ppm (560 mg m⁻³)

JP-OEL 50 ppm (280 mg m⁻³)

SE-LEVL 25 ppm (150 mg m⁻³)

SE-STEL 50 ppm (300 mg m⁻³)

UK-LTEL 100 ppm (566 mg m⁻³)

UK-STEL 150 ppm (850 mg m⁻³)

US-TWA 100 ppm (556 mg m⁻³)

UN No. 1299 **HAZCHEM Code** 3  **Conveyance classification** flammable liquid

Supply classification harmful

Risk phrases Flammable – Harmful by inhalation, in contact with skin and if swallowed (R10, R20/21/22)

Safety phrases Keep out of reach of children (if sold to general public) (S2)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 5.76 g kg⁻¹ (1).

LC₅₀ (2 hr) inhalation mouse 29 mg m⁻³ (2).

LD₅₀ intravenous mouse 1.18 mg kg⁻¹ (2).

Oral TD_{Lo} in one woman was reported as 560 mg kg⁻¹, causing kidney damage (3).

TC_{Lo} inhalation in one human subject was found to be 175 ppm, causing damage to eyes, pulmonary system and nose (4).

Irritancy

Can defat the skin, causing irritation and dermatitis (5).

Other effects

Other adverse effects (human)

Poisoning after ingestion is accompanied by local burning of the mouth, coughing, pulmonary oedema, coma and liver damage (6).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (7).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (8).

Other comments

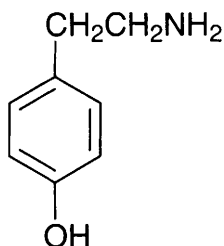
Reviews on human health effects, experimental toxicology, physico-chemical properties listed (9).

Toxicology has been reviewed (10).

References

1. *Pharmazie* 1959, **14**, 435.
2. *Toxicol. Appl. Pharmacol.* 1964, **6**, 360.
3. *Arch. Disease Childhood* 1953, **28**, 475.
4. *J. Ind. Hyg. Toxicol.* 1943, **25**, 282.
5. *HSE Toxic Substances Bulletin* 1984, **24**, 11.
6. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
7. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
8. *S.I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
9. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
10. Gosselin, R. E. et al (Eds.) *Clinical Toxicology of Commercial Products* 4th ed., 1976, Williams & Wilkins, Baltimore, MD, USA

T375 tyrosamine



$\text{C}_8\text{H}_{11}\text{NO}$

Mol. Wt. 137.18

CAS Registry No. 51-67-2

Synonyms 4-(2-aminoethyl)phenol; tyramine; 4-hydroxyphenethylamine; *p*- β -aminoethylphenol; α -(4-hydroxyphenyl)- β -aminoethane

EINECS No. 200-115-8

RTECS No. SJ 5950000

Uses Therapeutically as the hydrochloride as a sympathomimetic agent.

Occurrence In mistletoes, putrefied animal tissue, ripe cheese, wines and other fermented products (1,2).

Physical properties

M. Pt. 161°C B. Pt. 175-181°C at 8 mmHg

Solubility Water: 1 g l⁻¹ at 15°C. Organic solvents: benzene, ethanol

Ecotoxicity

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 27.6 ppm Microtox test (3).

Mammalian & avian toxicity

Acute data

Acute oral toxicity in Wistar rats > 2000 mg kg⁻¹ (4).

LD₅₀ intravenous mouse, rabbit 229, 300 mg kg⁻¹, respectively (5,6).

LD_{Lo} intraperitoneal mouse 800 mg kg⁻¹ (7).

LD_{Lo} subcutaneous cat, mouse 30, 225 mg kg⁻¹, respectively (8,9).

Sub-acute and sub-chronic data

No-observed-adverse-effect level (6 wk) in Wistar rat 2000 ppm in diet (180 mg kg⁻¹ day⁻¹) (4).

Metabolism and toxicokinetics

In humans the compound can be absorbed from the gastro-intestinal tract and can penetrate most organs, including the brain. It can be deaminated by monoamine oxidase types A and B in a variety of tissues, including the wall of the gastro-intestinal tract and the central nervous system (10-12).

It can be conjugated, and production of tyramine-O-sulfate as a urinary metabolite of a test dose has been used as a trait marker for some forms of depressive illness (13).

Genotoxicity

In vitro mouse lymphoma L5178Y cell assay without metabolic activation negative (14).

In vitro SOS chromatest using *Escherichia coli*, tyrosine nitrosated with nitrite gave a positive response in the absence of metabolic activation (15).

In vivo mouse bone marrow cells micronucleus test positive (16).

In vivo rat bone marrow cells chromosomal aberrations positive (17).

Other effects

Other adverse effects (human)

The potentially fatal consequences of ingesting tyrosamine whilst receiving therapy with monoamine oxidase inhibitors have been well documented (2,18).

In normal subjects, tyrosamine is rapidly inactivated by monoamine oxidase, but when the enzyme is inhibited, tyrosamine can cause hypertensive crises by its direct sympathomimetic actions (18).

Other comments

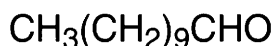
Human pharmacokinetics reviewed (10).

References

1. Vidal-Carou, M. et al *J. Food Compos. Anal.* 1989, **2**(3), 210-218.
2. da Prada, M. *Acta Psychiatr. Scand. Suppl.* 1990, **360**, 7-12.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. Til, H. P. et al *Food Chem. Toxicol.* 1997, **35**(3-4), 337-348.
5. *Acta Pharmacol. Toxicol.* 1976, **38**, 474.
6. Marhold, J. *Prehled Prumyslove Toxikologie; Organické Latky* 1986, Prague, Czechoslovakia.
7. *J. Physiol.* 1932, **76**, 224.
8. *Handbuch der Biologischen Arbeitsmethoden* 1935, **4**, 1412.

9. Barnes, C. D. et al (Eds.) *Drug Dosages in Laboratory Animals – A Handbook* 1973, Univ. California Press, Berkeley, CA, USA.
10. Bleck, P. R. *Klin. Pharmacol.* 1990, **3**, 44-49.
11. Durand, M. *Neurosci. Lett.* 1986, **72**(2), 174-178.
12. Elorriaga, C. et al *Biochem. Pharmacol.* 1990, **40**(3), 535-543.
13. Hale, A. S. et al *Lancet* 1989, **1**, 234-236.
14. McGregor, D. B. *Environ. Mol. Mutagen.* 1988, **11**(4), 523-544.
15. Ohshima, H. et al *Food Chem. Toxicol.* 1989, **27**(3), 193-203.
16. Fujie, K. et al *Mutat. Res.* 1990, **240**(1), 19-23.
17. Fujie, K. et al *Mutat. Res.* 1990, **240**(4), 281-288.
18. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK

U1 undecanal



$\text{C}_{11}\text{H}_{22}\text{O}$

Mol. Wt. 170.30

CAS Registry No. 112-44-7

Synonyms 1-decylaldehyde; hendecanal; hendecanaldehyde; undecylic aldehyde

EINECS No. 203-972-6

RTECS No. YQ 1500000

Occurrence In a variety of volatile oils from plants. In tobacco smoke and as an atmospheric pollutant (1).

Physical properties

M. Pt. -4°C B. Pt. 117°C at 18 mmHg Flash point 92°C Specific gravity 0.830 at 20°C with respect to water at 4°C Volatility v.p. 0.44 mmHg at 20°C ; v.den. 5.94

Environmental fate

Degradation studies

The long-term fate of undecanal present in sewage-contaminated groundwater has been reviewed (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat $>5 \text{ g kg}^{-1}$ (3).

LD₅₀ dermal rabbit $>5 \text{ g kg}^{-1}$ (3).

Other effects

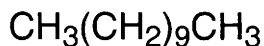
Any other adverse effects

The compound can increase the permeability of human lung fibroblasts *in vitro* (4) and demonstrate ciliotoxicity to cultured chicken embryo cells *in vitro* (5).

References

1. Yokouchi, Y. et al *Ko Kuritsu Kogai Ken Kyusho Kenkyu Hokoko* 1989, **123**, 91-97 (Japan.) (*Chem. Abstr.* 112, 83159p).
2. Thurman, E. M. et al *Environ. Sci. Technol.* 1988, **22**(2), 205-211.
3. *Food Cosmet. Toxicol.* 1973, **11**, 81.
4. Thelestam, M. et al *Toxicology* 1980, **15**, 203-217.
5. Petterson, B. et al *Toxicology* 1982, **23**, 41-55

U2 undecane



$\text{C}_{11}\text{H}_{24}$

Mol. Wt. 156.31

CAS Registry No. 1120-21-4

Synonyms hendecane; *n*-undecane

EINECS No. 214-300-6

RTECS No. YQ 1525000

Occurrence As an environmental pollutant. In essential oils and odours of a variety of plants and foods. In oil and coal liquors.

Physical properties

M. Pt. -26°C B. Pt. 195.6°C Flash point 60°C Specific gravity 0.7402 at 20°C with respect to water at 4°C

Volatility v.den. 5.4

Occupational exposure

UN No. 2330 HAZCHEM Code 3  Conveyance classification flammable liquid

Ecotoxicity

Invertebrate toxicity

The effects on environmental bacteria have been reviewed (1).

Environmental fate

Anaerobic effects

IC₅₀ Methanogens 0.61 mg l^{-1} (1).

Degradation studies

Anaerobic biodegradation can occur under methanogenic conditions (2).

Can be degraded by naturally occurring marine microorganisms within 20 days when present in No. 20 diesel oil (3).

Mammalian & avian toxicity

Acute data

LD₅₀ intravenous mouse 517 mg kg^{-1} (4).

Rats exposed to vapour for 8 hr at 20°C developed symptoms of acute central nervous system toxicity. NOEC 2411 ppm (5).

Symptoms of toxicity include narcosis (5,6).

Metabolism and toxicokinetics

After inhalation, the compound is distributed to tissues including the brain (5).

Irritancy

Irritant to eyes (species unspecified) (6).

Sensitisation

The compound can cause dermatitis (species unspecified) (6).

Other comments

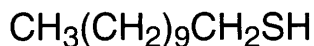
The effects on environmental bacteria have been reviewed (1).

Acute toxicity has been reviewed (7).

References

1. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, **63**(3), 198-207.
2. Sun, Y. et al *Haiyong YH* 1988, **19**(6), 518-524 (Ch.) (*Chem. Abstr.* **110**, 151103b).
3. Battersby, N. S. *Appl. Environ. Microbiol.* 1989, **55**(2), 433-439.
4. *J. Pharm. Sci.* 1978, **67**, 566.
5. Nilsen, O. G. et al *Pharmacol. Toxicol. (Copenhagen)* 1988, **62**(5), 259-266.
6. *BDH Hazard Data Sheets* BDH, Poole, Dorset, UK.
7. Jacobs, G. A. *Acute Toxic. Data* 1990, **1**(1), 57-58

U3 1-undecanethiol



$\text{C}_{11}\text{H}_{24}\text{S}$

Mol. Wt. 188.38

CAS Registry No. 5332-52-5

Occurrence In natural gas condensates and petroleum derivatives.

Mammalian & avian toxicity

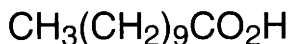
Acute data

LC₅₀ oral mouse 1138 mg kg⁻¹ day⁻¹ (based on food reduction values in 3-day feeding test at a 2% treatment rate) (1).

References

1. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1985, **14**(1), 111-129

U4 undecanoic acid



$\text{C}_{11}\text{H}_{22}\text{O}_2$

Mol. Wt. 186.29

CAS Registry No. 112-37-8

Synonyms 1-decanecarboxylic acid; hendecanoic acid; undecylic acid

EINECS No. 203-964-2

RTECS No. YQ 2275000

Physical properties

M. Pt. 28.5°C B. Pt. 228°C at 160 mmHg Flash point >110°C

Environmental fate

Degradation studies

Degraded by an anaerobic obligately syntrophic fatty acid-degrading acetogenic bacterium LDB1. The fermentation products included methane, acetic acid and propionic acid (1).

Biodegradation in activated sludge resulted in the formation of a lower fatty acid (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird, starling 100 mg kg⁻¹ (3).

LD₅₀ dermal rabbit 40 mg kg⁻¹ (4).

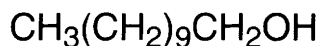
Irritancy

Dermal rabbit (24 hr) 150 mg caused mild irritation (5).

References

1. Zhao, Y. et al *Weishengwu Xuebao* 1991, 31(2), 133-138.
2. Nitsuma, T. et al *Tokoku Gakvin Daigaku Kogakubu Kenkyu Hokoku* 1988, 23(1), 57-60.
3. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, 12, 355-382.
4. *Acta Pharmacol. Toxicol.* 1961, 18, 141.
5. *Toxicol. Appl. Pharmacol.* 1972, 21, 369

U5 1-undecanol



C₁₁H₂₄O

Mol. Wt. 172.31

CAS Registry No. 112-42-5

Synonyms undecyl alcohol; hendecyl alcohol; Tip-Nip

EINECS No. 203-970-5

RTECS No. YQ 3155000

Physical properties

M. Pt. 11°C B. Pt. 146°C at 30 mmHg Flash point 112.22°C Specific gravity 0.820-0.840

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow 1.04 mg l⁻¹ (1).

Environmental fate

Degradation studies

Biodegradation in activated sludge resulted in the formation of the corresponding fatty acid (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 3000 mg kg⁻¹ (3).

Irritancy

Dermal rabbit (24 hr) 500 mg caused moderate irritation (4).

Other comments

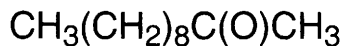
Toxicity reviewed (5).

References

1. Veith, G. D. *Can. J. Fish Aquat. Sci.* 1983, 40, 743.

2. Nitsuma, T. et al *Tohoku Gakuin Daigaku Kogakubu Kenkyu Nokoku* 1988, 23(1), 57-60.
3. *J. Ind. Hyg. Toxicol.* 1944, 26, 269.
4. *Food Cosmet. Toxicol.* 1978, 16, 637.
5. *BIBRA Toxicity Profile* 1991, British Industrial Biological Research Association, Carshalton, UK

U6 2-undecanone



$\text{C}_{11}\text{H}_{22}\text{O}$

Mol. Wt. 170.30

CAS Registry No. 112-12-9

Synonyms undecan-2-one; methyl nonyl ketone; nonyl methyl ketone

EINECS No. 203-937-5

RTECS No. YQ 2820000

Physical properties

M. Pt. 12°C B. Pt. 231-232°C Flash point 89°C (closed cup) Specific gravity 0.829 at 30°C

Partition coefficient $\log P_{\text{ow}}$ 4.09 Volatility v.den. 5.9

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird 100 mg kg⁻¹ (1).

LD₅₀ oral mouse, rat 3880, 5000 mg kg⁻¹, respectively (2,3).

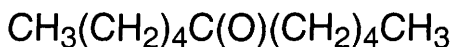
Legislation

The $\log P_{\text{ow}}$ value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (4).

References

1. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, 12, 355-382.
2. *Acta Pharm. Jugo.* 1962, 12, 79.
3. *Farm Chemicals Handbook* 1980, D200, Meister Publishing, Willoughby, OH, USA.
4. 1967 Directive on Classification, Packaging and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK

U7 6-undecanone



$\text{C}_{11}\text{H}_{22}\text{O}$

Mol. Wt. 170.30

CAS Registry No. 927-49-1

Synonyms undecan-6-one; diamyl ketone; pentyl ketone

EINECS No. 213-150-9

RTECS No. YQ 2828000

Physical properties

M. Pt. 14.6°C B. Pt. 288°C Flash point 88°C Specific gravity 0.831

Mammalian & avian toxicity

Acute data

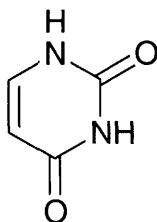
LD_{Lo} oral rat 1000 mg kg⁻¹ (1).

LD₅₀ intravenous mouse 117 mg kg⁻¹ (2).

References

1. *Clin. Toxicol.* 1980, **17**, 271.
2. *J. Pharm. Sci.* 1978, **67**, 566

U8 uracil



C₄H₄N₂O₂

Mol. Wt. 112.09

CAS Registry No. 66-22-8

Synonyms 2,4(1*H*,3*H*)-pyrimidinedione; 2,4-dihydroxypyrimidine; hybar X; pirod; 2,4-pyrimidinediol

EINECS No. 200-621-9

RTECS No. YQ 8650000

Uses In biochemical research.

Occurrence A pyrimidine derivative obtained by hydrolysis of nucleic acids.

Physical properties

M. Pt. 335°C

Solubility Water: 0.358% w/w at 25°C

Environmental fate

Degradation studies

Degraded by *Escherichia coli* B; the products included dihydrouracil, *N*-carbamoyl-β-alanine and β-alanine. The bacteria were able to utilise it as the sole nitrogen source (1).

Pseudomonas stutzeri was able to utilise uracil as sole source of nitrogen (2).

Uracil is catabolised in *Burkholderia cepacia* ATTC 25416 via a reductive pathway. The first pathway enzyme, dihydropyrimidine dehydrogenase, used NADPH as its nicotinamide cofactor. The second and third pathway enzymes are dihydropyrimidinase and *N*-carbamoyl-β-alanine amidohydrolase, respectively (3).

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal mouse 1513 mg kg⁻¹ (4).

Sub-acute and sub-chronic data

Weanling ♂ rats administered 3% uracil for 2, 4, 6, 10 and 16 wk induced hyperplasia (site unspecified) (5).

Carcinogenicity and chronic effects

Weanling ♂ rats administered 3% uracil for 2, 4, 6, 10 and 16 wk induced hyperplasia (site unspecified) (5).

References

1. Patel, B. N. et al *Microbios* 1987, **49**(199), 107-113.
2. West, T. P. *Microbios* 1990, **61**(247), 71-81.
3. West, T.P. *Arch. Microbiol.* 1997, **168**(3), 237-239.
4. *J. Pharmacol. Exp. Ther.* 1978, **207**, 504.
5. Debiec-Rychter, M. et al *Toxicol. Appl. Pharmacol.* 1990, **105**(2), 345-349

U9 uranium

U

U

Mol. Wt. 238.03

CAS Registry No. 7440-61-1

Synonyms uranium-238

EINECS No. 231-170-6

RTECS No. YR 3490000

Uses ^{235}U is used in atom and hydrogen bombs. ^{234}U and ^{235}U are used as nuclear fuel in power reactors.

Occurrence In pitchblende. Occurrence in Earth's crust $2 \times 10^{-5}\%$.

Physical properties

M. Pt. 1132°C B. Pt. 3818°C Specific gravity 18.95

Occupational exposure

DE-MAK 0.25 mg m⁻³ (inhalable fraction of aerosol)

US-TWA 0.2 mg m⁻³

US-STEL 0.6 mg m⁻³

UN No. 2979 (pyrophoric)

Supply classification very toxic

Risk phrases Very toxic by inhalation and if swallowed – Danger of cumulative effects (R26/28, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – When using do not eat, drink or smoke – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S20/21, S45)

Ecotoxicity

Invertebrate toxicity

LC₅₀ (48 hr) *Daphnia magna* 6 mg l⁻¹ (form unspecified) (1).

LOEC *Daphnia magna* 0.5 mg l⁻¹ (form unspecified) (1).

Bioaccumulation

Mytilus sp. contained 1.5 µg g⁻¹ ash, it was absorbed by gills and the digestive tract and excreted by the kidney (2).

Pseudomonas sp. EPS-5028 absorbed 55 mg g⁻¹ cell dry weight. Electron microscopy indicated that it accumulated intracellularly as needle-like fibrils (3).

Mammalian & avian toxicity

Acute data

LD₅₀ intravenous rabbit, guinea pig 0.1, 0.3 mg kg⁻¹, respectively (as uranium, form unspecified) (4).

LD₅₀ intravenous rat, mouse 1, 10-20 mg kg⁻¹, respectively (as uranium, form unspecified) (4).

Carcinogenicity and chronic effects

Osteosarcomas and lung cancers may occur in humans after inhalation of insoluble uranium, due to the effect of prolonged irradiation of the thorax (5).

Rats injected with metallic uranium in the bone marrow and chest wall developed sarcomas (6).

Teratogenicity and reproductive effects

Chronic uranium poisoning may inhibit reproduction and affect uterine and extrauterine development in experimental animals (5).

♂ Swiss mice (64 day) 0, 10, 20, 40 and 80 mg kg⁻¹ day⁻¹. Testicular function/spermatogenesis was not affected at any dose, as evidenced by normal testes and epididymis weights and normal spermatogenesis, whereas interstitial alterations and vacuolation of Leydig cells were seen at 80 mg kg⁻¹ day⁻¹. Although spermatogenesis was not affected by its administration, it produced a significant decrease in the pregnancy rate at 10, 20, 40 or 80 mg kg⁻¹ day⁻¹ (7).

Metabolism and toxicokinetics

Inhalation monkey, dog, rat (5 yr) 5 mg m⁻³ for 6 hr day⁻¹, 5 day wk⁻¹. It accumulated in the lungs and tracheobronchial lymph nodes. After 5 yr, monkey spleen contained 350 µg g⁻¹ and dog spleen contained 0.9 µg g⁻¹ (4).

Soluble uranium compounds are rapidly absorbed and are particularly injurious to the kidneys (5).

Approximately 20% of a dose in the bloodstream is deposited immediately in the kidney, followed by a 60% mobilisation of the dose to the urine in 24 hr. 10-30% of the dose is deposited in the bone (species unspecified) (4). Gastro-intestinal absorption in 10 normal healthy adult volunteers of both sexes 200-300 µg l⁻¹ uptake under these conditions averaged 0.6% (8).

Oral gavage ♂ Wistar rat 0.003-45 mg kg⁻¹. It was rapidly localised in the kidneys and bone following ingestion. Bone was found to be the primary tissue of deposition. Skeletal and kidney burdens closely paralleled each other from 15 min to 10 days after ingestion (9).

Genotoxicity

In vivo human sister chromatid exchanges and chromosomal aberrations were observed (5).

Other effects

Other adverse effects (human)

Insoluble uranium compounds are injurious to the lungs, due to the deposition of radioactive particles which are only cleared slowly (5).

15- and 25-yr-old assessments of the health of workers at a uranium plant failed to link exposure with any major kidney or blood diseases (10,11).

The insoluble compounds are only cleared slowly from the lungs, and chronic exposure may cause pulmonary fibrosis, pneumoconiosis. Changes to red and white blood cells and central nervous symptoms may also be observed (12,13).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (14).

Other comments

It is estimated that the average body burden of a 70 kg ICRP standard man is 100-125 µg (4).

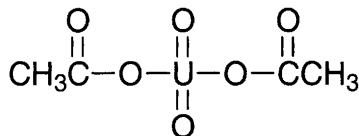
Reviews on human health effects, experimental toxicity, physico-chemical properties, epidemiology, workplace experience and environmental effects listed (15).

References

1. Poston, T. M. et al *Water, Air, Soil Pollut.* 1984, **22**(3), 289-298.
2. Chassard-Bouchard, C. *Oceanis* 1988, **14**(1), Gestion Ecol. Milieu Mar., 167-195.

3. Marques, A. M. et al *Appl. Microbiol. Biotechnol.* 1991, **35**(3), 406-410.
4. *Patty's Industrial Hygiene and Toxicology* 3rd rev. ed., 1981, **2A**, John Wiley & Sons, New York, NY, USA.
5. *Chemical Safety Data Sheets* 1991, **4b**, The Royal Society of Chemistry, London, UK.
6. Hueper, W. C. et al *J. Natl. Cancer Inst.* 1952, **13**, 291.
7. Llobet, J. M. et al *Fundam. Appl. Toxicol.* 1991, **16**(4), 821-829.
8. Wrean, M. E. et al *Radiat. Prot. Dosim.* 1989, **26**(1-4), 119-122.
9. LaTouche, Y. D. et al *Health Phys.* 1987, **53**(2), 147-162.
10. Mason, M. G. et al *HASL-58, Symposium on Occupational Health Experience and Practices in the Uranium Industry* 1958, New York, NY, USA.
11. Wing, J. F. et al *10th Ann. Meeting, Health Physics Soc.* 1963, CA, USA.
12. Boeglin, C. et al *Pharmacology and Toxicology of Uranium Compounds* 1949, **1**, National Nuclear Energy Series, McGraw-Hill, New York, NY, USA.
13. Tannenbaum, A. *Toxicology of Uranium* 1951, **23**, National Nuclear Energy Series, McGraw-Hill, New York, NY, USA.
14. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
15. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

U10 uranyl acetate



C₄H₆O₆U

Mol. Wt. 388.12

CAS Registry No. 541-09-3

Synonyms bis(acetato-O)dioxouranium; uranium oxyacetate; uranyl diacetate

EINECS No. 208-767-5

RTECS No. YR 3675000

Uses In dry copying inks. Activator in bacterial oxidation processes. Reagent for precipitating sodium.

Physical properties

M. Pt. loses 2 H₂O at 110°C **B. Pt.** 275°C (decomp.) **Specific gravity** 2.893 at 15°C

Solubility Water: 100 g l⁻¹

Occupational exposure

DE-MAK 0.25 mg m⁻³ (as U) (inhalable dust fraction)

UK-LTEL 0.2 mg m⁻³ (as U)

UK-STEL 0.6 mg m⁻³ (as U)

US-TWA 0.2 mg m⁻³ (as U)

US-STEL 0.6 mg m⁻³ (as U)

Supply classification very toxic

Risk phrases Very toxic by inhalation and if swallowed – Danger of cumulative effects (R26/28, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – When using do not eat, drink or smoke – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S20/21, S45)

Mammalian & avian toxicity

Teratogenicity and reproductive effects

Gavage pregnant Swiss mice 0, 5, 10, 25 or 50 mg kg⁻¹ on days 6-15 of gestation. Dose-related foetal toxicity, consisting primarily of reduced foetal body weight and body length, and an increased incidence of abnormalities

were observed. Malformations and developmental variations were noted at the 25 and 50 mg kg⁻¹. NOEL for foetotoxicity including teratogenicity was <5 mg kg⁻¹ day⁻¹ (1).
 Gavage ♂ and ♀ Swiss mice in mating study 0, 5, 10 and 25 mg kg⁻¹ day⁻¹. Embryo lethality could be observed in the 25 mg kg⁻¹ day⁻¹ group. Significant increases in the number of dead young litter⁻¹ were seen at birth and at day 4 of lactation in the 25 mg kg⁻¹ day⁻¹ group. The present results suggest that uranium dose not cause adverse effects on fertility, general reproductive parameters, or offspring survival at the concentration usually ingested by man (2).

Other effects

Any other adverse effects

Intravenous rabbits 0.8 mg kg⁻¹ induced acute renal failure, with recovery after 2 wk (3).

Subcutaneous rats and mice (dose unspecified) suffered severe lesions in liver and kidney (4).

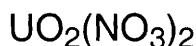
Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (5).

References

1. Domingo, J. L. et al *Bull. Environ. Contam. Toxicol.* 1987, **39**(1), 168-174.
2. Paternain, J. L. *Ecotoxicol. Environ. Saf.* 1989, **17**(3), 291-296.
3. Yonemura, K. *Jpn. J. Nephrol.* 1986, **28**(9), 1221-1227.
4. Domingo, J. L. et al *Toxicology* 1989, **55**(1-2), 143-152.
5. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

U11 uranyl nitrate



N₂O₈U

Mol. Wt. 394.04

CAS Registry No. 10102-06-4

Synonyms uranyl dinitrate; (T-4)-bis(nitrato-O)dioxouranium; dinitratodioxouranium; uranium nitrate oxide

EINECS No. 233-266-3

RTECS No. YR 3805000

Physical properties

M. Pt. 60.2°C **B. Pt.** 118°C **Specific gravity** 2.807 at 13°C

Solubility Water: 33 g l⁻¹ at 100°C

Occupational exposure

DE-MAK 0.25 mg m⁻³ (as U) (inhalable dust fraction)

UK-LTEL 0.2 mg m⁻³ (as U)

UK-STEL 0.6 mg m⁻³ (as U)

US-TWA 0.2 mg m⁻³ (as U)

US-STEL 0.6 mg m⁻³ (as U)

UN No. 2981 (solid)

UN No. 2980 (hexahydrate, solution)

Supply classification very toxic

Risk phrases Very toxic by inhalation and if swallowed – Danger of cumulative effects (R26/28, R33)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – When using do not eat, drink or smoke – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S20/21, S45)

Other effects

Any other adverse effects

A 0.5 mg perfusion into the early proximal tubule produced a 16-30% reduction in the nephron filtrations rate measured in both distal and proximal reabsorption (species unspecified) (1).

Intraperitoneal rats 2 or 0.8 mg kg⁻¹, a decrease in bone formation was observed (2).

♂ Sprague Dawley rats 5, 15 and 30 mg kg⁻¹ induced weight loss, polydipsia and polyuria 24 hr after injection (3).

Legislation

Included in Schedule 4 (Release into the Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (4).

References

1. Peterson, O. W. et al *Kidney Int.* 1989, **36**(6), 1037-1044.
2. Ubios, A. M. et al *Environ. Res.* 1991, **54**(1), 17-23.
3. Lim, I. K. et al *Yonsei Med. J.* 1987, **28**(1), 38-48.
4. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

U12 urea



CH₄N₂O

Mol. Wt. 60.06

CAS Registry No. 57-13-6

Synonyms Benural 70; B-I-K; carbamide; carbonyl diamide; isourea; Urevert

EINECS No. 200-315-5

RTECS No. YR 6250000

Uses Fertilizer. In animal feeds. In ammoniated dentifrices. Diuretic.

Occurrence Product of protein metabolism excreted in urine.

Physical properties

M. Pt. 132.7°C **B. Pt.** decomp. **Specific gravity** 1.335

Solubility Water: 1 kg l⁻¹. Organic solvents: ethanol, methanol, glycerol

Ecotoxicity

Invertebrate toxicity

LOEC *Entosiphon sulcatum* 29 mg l⁻¹ (1).

LOEC *Pseudomonas putida*, *Scenedesmus quadricauda* >10,000 mg l⁻¹ (1).

EC₅₀ (5 min) *Photobacterium phosphoreum* 23,914 ppm Microtox test (2).

Environmental fate

Nitrification inhibition

No inhibition of ammonia oxidation by *Nitrosomonas* sp. at 100 mg l⁻¹ (3).

Degradation studies

After 5 days at 35°C ¹⁴C₂ was 70.1% of the ¹⁴C-urea initially applied to anaerobic suspended soil (4).

Biodegradation in river water at 1-15 mg l⁻¹, degradation rate is negligible below 8°C for up to 14 days, degradation at 20°C within 4-6 days (5).

Hebeloma spp. and *Laccaria* spp. are able to degrade urea with urease (6).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 8471 mg kg⁻¹ (7).

LD₅₀ subcutaneous rat, mouse 8200, 9200 mg kg⁻¹, respectively (8).

LD₅₀ intravenous mouse, rat 4600, 5300 mg kg⁻¹, respectively (8).

Metabolism and toxicokinetics

In humans, it is rapidly absorbed from the gastro-intestinal tract, but causes gastro-intestinal irritation. It is distributed into extracellular and intracellular fluids, including lymph, bile and blood, and can cross the placenta and penetrate the eye. It is excreted unchanged in the urine (9).

Genotoxicity

In vitro DNA alkaline unwinding assay without metabolic activation positive (10).

In vitro mouse lymphoma L5178Y tk⁺/tk⁻ without metabolic activation positive (11).

Other effects

Other adverse effects (human)

Rapid intravenous injection of solutions of urea can cause haemolysis and venous thrombosis or phlebitis at the site of injection (9).

Other comments

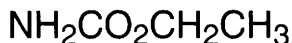
Reviews on human health effects, environmental effects, experimental toxicity, ecotoxicology and exposure levels listed (12).

Interaction of urea with soil clay reviewed (13).

References

1. Bringmann, G. et al *Water Res.* 1980, **14**, 231-241.
2. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
3. Hockenbury, M. R. et al *Res. J. Water Pollut. Control Fed.* 1977.
4. Scheunert, I. et al *Chemosphere* 1987, **16**(5), 1031-1041.
5. Evans, W. H. et al *Water Res.* 1973, **7**, 975-985.
6. Hutchinson, L. J. *Can. J. Bot.* 1990, **68**(7), 1522-1530.
7. *Gig. Sanit.* 1986, **51**(6), 8.
8. *Oyo Yakuri* 1977, **13**, 749.
9. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
10. Garberg, P. et al *Mutat. Res.* 1988, **203**, 155-176.
11. Wangenheim, J. et al *Mutagenesis* 1988, **3**(3), 193-205.
12. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
13. Banerjee, B. K. *Cent. Glass Ceram. Res. Inst. Bull.* 1987, **34**(2), 38-44.

U13 urethane



$\text{C}_3\text{H}_7\text{NO}_2$

Mol. Wt. 89.09

CAS Registry No. 51-79-6

Synonyms ethyl carbamate; ethyl urethane; leucethane; pracarbamin; urethan

EINECS No. 200-123-1

RTECS No. FA 8400000

Uses In molten form, solvent for organic materials. Intermediate in organic synthesis. Antineoplastic. Anaesthetic (veterinary).

Physical properties

M. Pt. 49°C **B. Pt.** 184°C **Flash point** 92°C **Specific gravity** 0.9862 **Volatility** v.p. 10 mmHg at 77.8°C ;
v.den. 3.07

Solubility Water: 2 kg l⁻¹. Organic solvents: chloroform, diethyl ether, ethanol, glycerol

Occupational exposure

Supply classification toxic

Risk phrases May cause cancer (R45)

Safety phrases Restricted to professional users – Avoid exposure – obtain special instruction before use – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S53, S45)

Ecotoxicity

Invertebrate toxicity

LC₅₀ *Xenopus laevis* 5580 mg l⁻¹ (1).

EC₅₀ *Xenopus laevis* 1800 mg l⁻¹ (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird, starling 100 mg kg⁻¹ (2).

LD₅₀ oral mouse 2500 mg kg⁻¹ (3).

LD₅₀ intraperitoneal rat, mouse 1500, 1539 mg kg⁻¹, respectively (4,5).

LD₅₀ subcutaneous mouse 1750 mg kg⁻¹ (6).

LD₅₀ intramuscular rat 400 mg kg⁻¹ (7).

Carcinogenicity and chronic effects

Oral ♂, ♀ Swiss albino mice (66 wk) 0.4% in drinking water. A 100% incidence of multiple lung adenomas was observed (8).

Oral ♂, ♀ outbred albino CTM mice (60-80 wk) 0.4% in drinking water. Lung adenomas, lymphosarcomas, liver angiomas and Harderian gland tumours were observed (9).

Oral ♀ Sprague Dawley rats (19 month) 0.1% in drinking water. 7 malignant lymphomas; 11 haemangomas or haemangiosarcomas of the liver, spleen or uterus; 7 hepatomas; 10 adrenal cortex adenomas; and 4 fibrosarcomas of the mesentery or uterus were seen (10).

Dermal ♂ and ♀ HR/De mice (14-15 month), 40% urethane solution in ethylene glycol on the interscapular area. Hairless mice had a tumour incidence of 43/51, hairless mice had an incidence of 30/40. A high incidence of epidermoid carcinoma 17/48 was observed only in hairless mice (11).

Subcutaneous Swiss albino mice (14 wk) 1 mg as a suspension in gelatin, 24 hr post-partum. Malignant lymphomas and pulmonary adenomas were observed (12).

Subcutaneous C57BL mice 1 mg g⁻¹ body weight 1 × wk⁻¹ for 8 wk produced thymic lymphomas in 12/12 treated animals (13).

Subcutaneous 7-day-old dd/I mice (26 wk) 1 mg g⁻¹ 1 × wk for 4 wk⁻¹. Thymic lymphomas were seen in 70% of treated animals at 11 wk, lung adenomas were seen in 90% at the same age, and Harderian gland tumours were seen in 44% at 26 weeks. Six liver tumours were also observed (14).

Teratogenicity and reproductive effects

In vitro rat and *in vivo* animal (species unspecified) teratogenic at ≥100 µg ml⁻¹ (15).

Metabolism and toxicokinetics

When given to rats and pregnant mice it is rapidly and evenly distributed throughout the body and is found in the body fluids of the rats and of the mouse fetuses (16).

In mice, ~90% of the administered dose is excreted within 24 hr as CO₂ in the expired air, ~6% remains in the body and 6% is excreted in the urine (17).

In rats, rabbits and humans, the urinary excreted products are: urethane (0.5-1.7%), *N*-hydroxyurethane (0.02-0.15%), acetyl-*N*-hydroxyurethane (0.1-0.6%), ethyl mercapturic acid (0.1-0.2%) and *N*-acetyl-*S*-ethoxycarbonylcysteine (0.9-2.1%) (18).

N-hydroxy derivative of ethyl carbamate, *N*-hydroxyvinyl carbamate, and the epoxy derivative of ethyl carbamate were produced *in vitro* on incubation with rat lung microsomes, but not with rat microsomes, from liver, kidney and brain (19).

The results of experiments using catalytic markers indicate that urethane is metabolised by cytochrome P₄₅₀ (CYP 2E1) and carboxyesterase (hydrolase A) in mouse liver microsomes (20).

Genotoxicity

Salmonella typhimurium TA98, TA100 with and without metabolic activation negative (21).

Drosophila melanogaster somatic mutation and recombination test. Induced single spots and twin spots in a dose-dependent manner. The twin spots indicate a recombinogenic activity (22).

LacZ transgenic mice were given a single intraperitoneal injection of urethane (900 mg kg⁻¹) followed by a 14 or 16 day expression period. Mutation frequency in the lung and liver increased twofold; increases in mutation frequency in the spleen and bone marrow were also observed. Bone marrow micronucleus assays showed an eight fold increase in micronucleated polychromatic erythrocytes (23).

Other effects

Any other adverse effects

Aspartate carbamoyl transferase activity of mouse liver and lung is inhibited *in vivo*, but not *in vitro* (24,25).

In rats, it showed mostly toxic effects on heart function (26).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (27).

Other comments

Can occur as a result of the reaction of ammonia and diethyl pyrocarbonate added at levels of 10 µg l⁻¹ in certain beverages at <pH 4.0.

Toxicity reviewed (28).

Reviews on human health effects, experimental toxicity, epidemiology, workplace experience, physico-chemical properties and environmental effects listed (29).

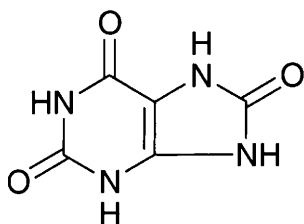
Developmental toxicity, metabolism, mutagenicity, carcinogenicity, biological activity and possible reaction pathways reviewed (30-34).

References

1. Dawson, D. A. et al *Drug Chem. Toxicol.* 1989, **12**(1), 67-75.
2. Schafer, E. W. *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
3. *Arzneim.-Forsch.* 1959, **9**, 595.

4. *Cancer Res.* 1966, **26**, 1448.
5. *Prog. Mutat. Res.* 1981, **1**, 682.
6. *Naunyn-Schmeideberg's Arch. Exp. Pathol. Pharmacol.* 1936, **182**, 348.
7. *Z. Krebsforsch. Klin. Onkol.* 1975, **84**, 227.
8. Toth, B. et al *Brit. J. Cancer* 1961, **15**, 322-326.
9. Della Porta, G. et al *Tumori* 1963, **49**, 413-428.
10. Adenis, L. et al *C. R. Soc. Biol. (Paris)* 1968, **162**, 458-461.
11. Deringer, M. K. *J. Natl. Cancer Inst.* 1962, **29**, 1107-1121.
12. Pietra, G. et al *Cancer* 1961, **14**, 308-317.
13. Doell, R. G. et al *Nature (London)* 1962, **194**, 588-589.
14. Matsuyama, M. et al *Brit. J. Cancer* 1970, **24**, 312-317.
15. Schmid, B. P. et al *Altern. Methods Toxicol.* 1987, 5(In Vitro Toxicol.), 179-187.
16. Boyland, E. et al *Biochem. J.* 1949, **44**, 528-531.
17. Bryan, C. E. et al *J. Biol. Chem.* 1949, **177**, 941-950.
18. Boyland, E. et al *Biochem. J.* 1965, **94**, 198-208.
19. Gupta, R. et al *Toxicol. Lett.* 1989, **45**(1), 49-53.
20. Lee, R. P. et al *Drug Metab. Dispos.* 1998, **26**(1), 60-65.
21. Khydooley, I. et al *Arch. Geschwulstforsch.* 1987, **57**(6), 453-462.
22. Froelich, A. et al *Mutat. Res.* 1990, **244**(3), 201-208.
23. Williams, C. V. et al *Mutagenesis* 1998, **13**(2), 133-137.
24. Giri, C. P. et al *Indian J. Exp. Biol.* 1968, **6**, 21-23.
25. Kaye, A. M. *Cancer Res.* 1968, **28**, 1041-1046.
26. Hoffman, P. et al *Wiss. Z. Ernst-Moritz-Arndt-Univ. Greifsw., Med. Reihe* 1988, **27**(2-3), 81-84.
27. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
28. *BIBRA Toxicity Profile* 1991, British Industrial Biological Research Association, Carshalton, UK.
29. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium.
30. Zimmerhi, B. et al *Mutat. Res.* 1991, **259**(3-4), 325-350.
31. Zhao, G. et al *Spipin Yu Fajiao Gongye* 1988, (5), 70-72.
32. Collins, T. F. X. et al *Toxicol. Ind. Health* 1989, **5**(6), 1045-1060.
33. Schlatter, J. et al *Food Chem. Toxicol.* 1990, **28**(3), 205-211.
34. *IARC Monograph* 1974, **7**, 111

U14 uric acid



C₅H₄N₄O₃

Mol. Wt. 168.11

CAS Registry No. 69-93-2

Synonyms 7,9-dihydro-1H-purine-2,6,8(3H)-trione; lithic acid; 2,6,8-trihydroxypurine; 2,6,8-trioxopurine

EINECS No. 200-720-7

RTECS No. YU 7050080

Occurrence Chief end-product of nitrogenous metabolism in birds and reptiles. Present in urine of carnivorous animals.

Physical properties

M. Pt. >300°C Specific gravity 1.89

Solubility Water: 64.5 mg l⁻¹ at 37°C. Organic solvents: glycerol

Environmental fate

Degradation studies

BOD₅ standard dilute sewage 0.300 mg O₂ l⁻¹ (1).

Genotoxicity

Inhibited mitotic rate of phytohaemagglutinin-stimulated human lymphocytes (2).

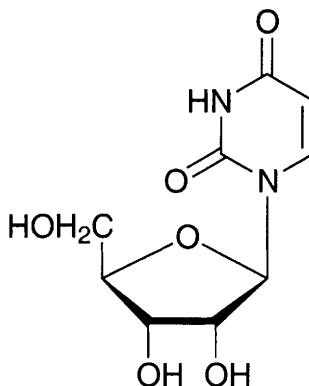
Other comments

Metabolism and nephropathy reviewed (3,4).

References

1. Meissner, B. *Wasser.-Wasser*. 1954, 4, 166.
2. *Cytobios* 1971, 4(14), 87-91.
3. Conger, J. D. *Med. Clin. North Am.* 1990, 74(4), 859-871.
4. Williams, A. W. et al *Semin. Nephrol.* 1990, 10(1), 9-14

U15 uridine



C₉H₁₂N₂O₆

Mol. Wt. 244.20

CAS Registry No. 58-96-8

Synonyms Uridin; 1-β-D-ribofuranosyluracil; uracilriboside

EINECS No. 200-407-5

RTECS No. YR 1450000

Occurrence Nucleoside widely distributed in nucleic acids.

Physical properties

M. Pt. 165°C

Solubility Water: soluble

Environmental fate

Abiotic removal

Ultra-violet radiation, 254 nm, in aqueous solution of phosphinic acid leads to formation of the corresponding dihydropyrimidine structures (1).

Lunar soil is an effective catalyst in the photolysis of uridine (2).

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal mouse 5100 mg kg⁻¹ (3).

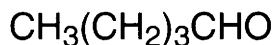
Other comments

Anti-tumour activity and separation of uridine-requiring auxotrophic mutant reviewed (4,5).

References

1. Yakoulev, D. Y. et al *Bioorg. Khim.* 1991, 17(6), 857-859.
2. Kuzicheva, E. A. *Zh. Evol. Biokhim. Fiziol.* 1987, 23(1), 3-8.
3. *Russ. Pharmacol. Toxicol.* 1977, 40, 66.
4. Klubes, P. et al *Pharmacol. Ther.* 1989, 41(1-2), 289-302.
5. Kusano, T. et al *Tanpakushitsu Kakusan Koso* 1991, 36(13), 2131-2133

v1 valeraldehyde



C₅H₁₀O

Mol. Wt. 86.13

CAS Registry No. 110-62-3

Synonyms pentanal; valeral; valerianic aldehyde; valeric aldehyde; *n*-valeraldehyde

EINECS No. 203-784-4

RTECS No. YV 3600000

Uses In flavouring compounds. Resin chemistry. Rubber accelerators.

Physical properties

M. Pt. -91°C **B. Pt.** 102-103°C **Flash point** 12°C **Specific gravity** 0.8095 at 20°C with respect to water at 4°C

Volatility v.p. 50 mmHg at 25°C ; v.den. 3.0

Solubility Organic solvents: miscible with many organic solvents

Occupational exposure

FR-VME 50 ppm (175 mg m⁻³)

US-TWA 50 ppm (176 mg m⁻³)

UN No. 2058 HAZCHEM Code 3ME **Conveyance classification** flammable liquid

Ecotoxicity

Fish toxicity

LC₅₀ (duration unspecified) fathead minnow 0.144 mg l⁻¹ (1).

LC₅₀ (14 day) guppy 0.338 mg l⁻¹ (2).

Environmental fate

Degradation studies

Wastewater treatment activated sludge after 6 hr 12.7% of ThOD, 12 hr 16.5% of ThOD, 24 hr 17.8% of ThOD (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 5.66 ml kg⁻¹ (4).

LD₅₀ oral mouse 6.4-12.8 mg kg⁻¹ (5).

Genotoxicity

Salmonella typhimurium TA1535 with metabolic activation positive, without metabolic activation negative (6).

Other comments

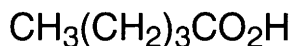
Toxicity reviewed (7).

Reviews on human health effects, experimental toxicity and workplace experience listed (8).

References

1. Protic, M. et al *Aquatic Toxicol.* 1989, **14**, 47-64.
2. Deneer, J. W. et al *Aquatic Toxicol.* 1988, **12**, 185-192.
3. Gerhold, R. M. et al *Res. J. Water Pollut. Control Fed.* 1966, **38**(4), 562.
4. Smyth, H. F. et al *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 470.
5. Patty, F. A. *Industrial Hygiene and Toxicology* 1967, **2**, Interscience Publishers, New York, NY, USA.
6. Ono, Y. et al *Water Sci. Technol.* 1991, **23**, 329-338.
7. *BIBRA Toxicity Profile* 1991, British Industrial Biological Research Association, Carshalton, UK.
8. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

v2 valeric acid



C₅H₁₀O₂

Mol. Wt. 102.13

CAS Registry No. 109-52-4

Synonyms pentanoic acid; 1-butanecarboxylic acid; propylacetic acid; valerianic acid

EINECS No. 203-677-2

RTECS No. YV 6100000

Uses Intermediate in perfumery.

Physical properties

M. Pt. -34.5°C **B. Pt.** 186-187°C **Flash point** 88°C **Specific gravity** 0.939 at 20°C with respect to water at 4°C **Partition coefficient** log P_{ow} 1.39 **Volatility** v.p. 0.15 mmHg at 20°C ; v.den. 3.52

Solubility Water: soluble in 30 parts water. Organic solvents: ethanol, diethyl ether

Occupational exposure

Supply classification corrosive

Risk phrases Causes burns (R34)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Wear suitable protective clothing – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S26, S36, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow 77 mg l⁻¹ (1).

LC₅₀ (24 hr) bluegill sunfish 5000 mg l⁻¹ (as Na salt) (2).

Invertebrate toxicity

LC₅₀ (48 hr) *Daphnia pulex*, *Daphnia magna* 45 mg l⁻¹ (3).

LC₁₀₀ (duration unspecified) *Chlorella pyrenoidosa* 280 mg l⁻¹ (4).

Environmental fate

Degradation studies

BOD₅ standard dilute sewage 1.06 mg O₂ l⁻¹ (5).

BOD₅ activated sludge 20°C (1-5 day) 333 mg O₂ l⁻¹, acclimated 15 days, 99% removed (6).

Alcaligenes denitrificans isolated from sewage sludge degraded 18mm over ten 48 hr runs (7).

Abiotic removal

Adsorption on activated carbon 0.159 g g⁻¹ (8).

Mammalian & avian toxicity

Acute data

LD₅₀ intravenous mouse 1290 mg kg⁻¹ (9).

LD₅₀ oral rat >400 mg kg⁻¹ (10).

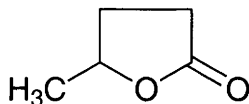
Other comments

Reviews on human health effects, experimental toxicology and physico-chemical properties listed (11).

References

1. Vincent, R. M. et al *Acute Toxicity of Selected Organic Compounds to Fathead Minnows* 1976, EPA-600/3-76-097.
2. Dowden, B. F. *Proc. LA Acad. Sci.* 1970, **23**, 77.
3. Freeman, L. *Sewage Ind. Wastes* 1953, **25**(7), 845.
4. Verschuere, K. *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, Van Nostrand Reinhold, New York, NY, USA.
5. Meissner, B. *Wasser.-Wasser.* 1954, **4**, 166.
6. Ludzack, F. J. et al *Res. J. Water Pollut. Control Fed.* 1960, **32**, 1173.
7. Caunt, P. et al *Appl. Microbiol. Biotechnol.* 1987, **25**(5), 453-458.
8. Guisti, D. M. et al *Res. J. Water Pollut. Control Fed.* 1974, **46**(5), 947-965.
9. Oro, L. et al *Acta Pharmacol. Toxicol.* 1961, **18**, 141.
10. Patty, F. A. *Industrial Hygiene and Toxicology* 1967, **2**, Interscience Publishers, New York, NY, USA.
11. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

v3 γ -valerolactone



$C_5H_8O_2$

Mol. Wt. 100.12

CAS Registry No. 108-29-2

Synonyms 4-valerolactone; 4-methylbutyrolactone; γ -pentalactone; 4-pentanoline; dihydro-5-methyl-2(3H)-furanone; 4-hydroxypentanoic acid lactone; 4-hydroxyvaleric acid lactone; valerolactone; tetrahydro-5-methyl-2-furanone

EINECS No. 203-569-5

RTECS No. LU 3580000

Physical properties

M. Pt. -31°C B. Pt. $207\text{--}208^{\circ}\text{C}$ Flash point 81°C Specific gravity 1.057

Ecotoxicity

Fish toxicity

Threespine stickleback, steelhead trout and sockeye salmon exposed to 2 mg l^{-1} in a 24 hr static bioassay suffered no ill-effects. Test conditions: artesian well water; total hardness $67\text{--}120\text{ mg l}^{-1}$; methyl orange alkalinity $151\text{--}183\text{ mg l}^{-1}$; total dissolved solids $160\text{--}175\text{ mg l}^{-1}$ and pH 7.1 (1).

Invertebrate toxicity

Toxicity testing using *Azospirillum brasilense*, *Proteus mirabilis* swarming inhibition inhibited by 1.2 mg ml^{-1} and 40 mg ml^{-1} , respectively. *Bacillus thuringiensis* growth inhibition at concentrations of 100 mg l^{-1} (2).

Other effects

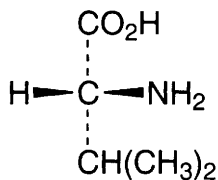
Other adverse effects (human)

Major urinary metabolite in shoe factory workers exposed to hexane. Toxic polyneuropathy was attributed to tetrahydro-5-methyl-2-furanone exposure (3).

References

1. *Lethal Effects of 2014 Chemicals Upon Sockeye Salmon, Steelhead Trout and Threespine Stickeback* 1989, US EPA 560/6-89-001, PB 89-156715, Washington, DC, USA.
2. Lenz, P. et al *Toxic. Assess.* 1989, 4(1), 43-52.
3. Governa, A. et al *J. Toxicol. Environ. Health* 1987, 20(3), 219-228

V4 D-valine



$\text{C}_5\text{H}_{11}\text{NO}_2$

Mol. Wt. 117.15

CAS Registry No. 640-68-6

Synonyms (R)-valine

EINECS No. 211-368-9

RTECS No. YV 9360000

Physical properties

M. Pt. 295-297°C (sublimes)

Solubility Water: soluble in water. Organic solvents: benzene, diethyl ether, ethanol

Other effects

Other adverse effects (human)

It inhibits fibroblasts proliferation in a culture of human endometrial stromal cells (1).

Other comments

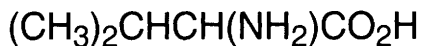
Stimulated the division of *Tetrahymena pyriformis* (2).

Utilised by *Halobacterium halobium* V0107H (3).

References

1. Frauli, M. et al *Arch. Gynecol. Obstet.* 1987, **241**(2), 87-96.
2. Darvas, Z. et al *Biosci. Rep.* 1987, **7**(10), 757-760.
3. Tanaka, M. et al *Viva Origino* 1991, **18**(3), 109-117.

V5 DL-valine



$\text{C}_5\text{H}_{11}\text{NO}_2$

Mol. Wt. 117.15

CAS Registry No. 516-06-3

Synonyms DL-α-aminoisovaleric acid

EINECS No. 208-220-0

Physical properties

M. Pt. 298°C (decomp.) B. Pt. sublimes Specific gravity 1.316

Solubility Water: 74.4 g l⁻¹ at 25°C. Organic solvents: benzene, diethyl ether, ethanol

Environmental fate

Nitrification inhibition

~50% inhibition of ammonia oxidation in *Nitrosomonas* sp. at 1.8 mg l⁻¹ (1).

68% inhibition of nitrogen dioxide utilisation by *Nitrobacter* sp. at 117 mg l⁻¹ (2).

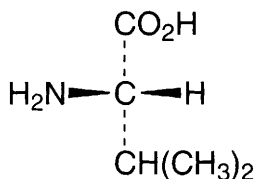
Other comments

Identified in the larval form of *Hydratigera balaniceps* (3).

References

1. Clark, C. et al *J. Bacteriol.* 1967, **93**, 1309.
2. Richardson, M. *Nitrification Inhibition in the Treatment of Sewage* 1985, The Royal Society of Chemistry, London, UK.
3. Malhotra, S. K. et al *Indian J. Parasitol.* 1987, **11**(1), 83

V6 L-valine



C₅H₁₁NO₂

Mol. Wt. 117.15

CAS Registry No. 72-18-4

Synonyms α-aminoisovaleric acid; (S)-valine

EINECS No. 200-773-6

RTECS No. YV 9361000

Uses Essential amino acid for human and mammalian nutrition.

Occurrence In fibrous proteins.

Physical properties

M. Pt. 295-300°C (sublimes) Specific gravity 1.230

Solubility Water: 88.5 g l⁻¹ at 25°C

Environmental fate

Nitrification inhibition

50% inhibition of ammonia oxidation in pure culture at 1.8 mg l⁻¹ (1).

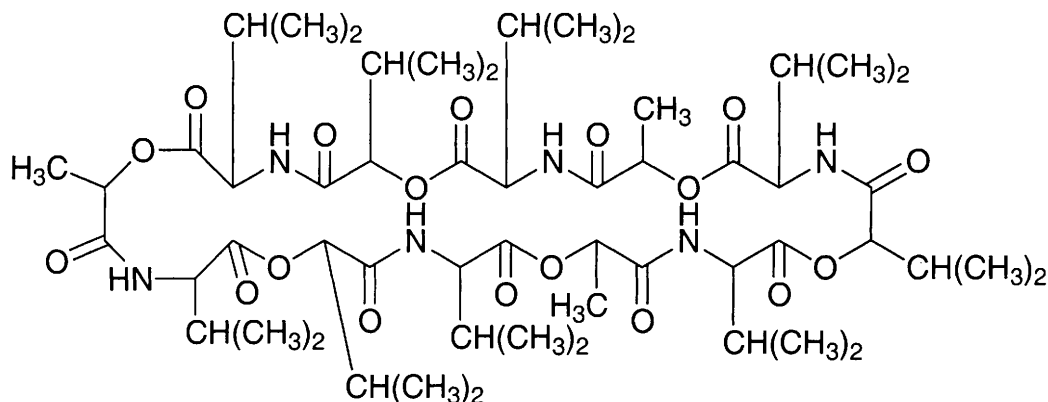
Genotoxicity

In vitro Chinese hamster ovary cells sister chromatid exchanges, chromosomal aberrations negative (2).

References

1. Richardson, M. L. *Nitrification Inhibition in the Treatment of Sewage* 1985, The Royal Society of Chemistry, London, UK.
2. Rosenkranz, H. S. et al *Environ. Mol. Mutagen.* 1990, **16**, 149-177

v7 valinomycin



$C_{54}H_{90}N_6O_{18}$

Mol. Wt. 1111.34

CAS Registry No. 2001-95-8

EINECS No. 217-896-6

RTECS No. YV 9468000

Uses Insecticide. Nematocide.

Occurrence Produced by some soil microorganisms such as *Actinomycetes* and *Streptomyces fulvissimus* (1).

Physical properties

M. Pt. 190°C

Solubility Organic solvents: acetone, benzene, chloroform, diethyl ether, light petroleum

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 4 mg kg⁻¹ (2).

LD₅₀ oral mouse 2500 µg kg⁻¹ (3).

LD₅₀ dermal rabbit 5 mg kg⁻¹ (2).

LD₅₀ intraperitoneal rat 800 µg kg⁻¹ (2).

LD₅₀ subcutaneous mouse 4140 µg kg⁻¹ (3).

Other effects

Any other adverse effects

Toxic to cultured rat hepatocytes at 50 µM after 8 hr incubation (4).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (5).

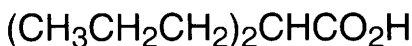
Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (6).

References

1. Heisey, R. M. et al *ACS Symp. Ser.* 1988, **380**(Biol. Act. Nat. Prod.: Potential Use Agric.), 65-78.
2. *Drug Chem. Toxicol.* 1985, **8**, 451.
3. Korzysko, T. et al (Eds.) *Antibiotics: Origin, Nature and Properties* 1978, American Society for Microbiology, Washington, DC, USA.
4. Mereish, K. A. et al *Med. Sci. Res.* 1989, **17**(20), 869-871.

5. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
6. S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations 1991, HMSO, London, UK

v8 valproic acid



C₈H₁₆O₂

Mol. Wt. 144.21

CAS Registry No. 99-66-1

Synonyms 2-propylpentanoic acid; Depakine; dipropylacetic acid; DPA; 2-propylvaleric acid

EINECS No. 202-777-3

RTECS No. YV 7875000

Uses Anticonvulsant.

Physical properties

B. Pt. 221-222°C, 220°C (98%) Flash point 111°C Specific gravity 0.922 at 0°C with respect to water at 4°C

Partition coefficient log P_{ow} 2.75

Solubility Water: very slightly soluble. Organic solvents: acetone, diethyl ether, ethanol, methanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, guinea pig, mouse 670, 824, 1098 mg kg⁻¹, respectively (1-3).

LD₅₀ subcutaneous mouse 860 mg kg⁻¹ (2).

LD₅₀ intraperitoneal mouse, rat 470, 704 mg kg⁻¹, respectively (4,5).

LD₅₀ intravenous mouse 509 mg kg⁻¹ (5).

Teratogenicity and reproductive effects

Gavage Sprague-Dawley CD rats 0, 150, 200, 300, 400 and 600 mg kg⁻¹. The 600 mg kg⁻¹ dose was maternally toxic and produced 100% embryonic resorption. The 400 mg kg⁻¹ dose was maternally toxic, maternal weight gain was reduced, no deaths occurred; 52% of all embryos were resorbed. Among survivors 49% were malformed, foetal weight was reduced by 43%. Defects observed were ectrodactyly, hydronephrosis, cardiovascular defects, hypoplastic bladder, rib and vertebral defects. The 300 mg kg⁻¹ dose produced fewer defects, larger foetuses, and no increase in resorptions; defects were primarily cardiovascular, rib and vertebral. The 200 mg kg⁻¹ dose produced no reduction in foetal weight, no increase in resorptions and a few defects, which were hydronephrosis, cardiovascular abnormalities and rib defects, primarily wavy ribs (6).

Oral rats 200-800 mg kg⁻¹ on days 8-17 of gestation. Increasing maternal toxicity at the higher doses with 100% maternal lethality at 800 mg kg⁻¹. An increased incidence of foetal resorptions at 600 mg kg⁻¹. Foetal examination on gestational day 20 revealed dose-dependent foetal growth retardation as evidenced by decreased foetal growth weight and length as well as underossification of the axial and appendicular skeleton. Abnormal vertebrae, ribs and craniofacial dysmorphism also increased with higher doses (7).

Valproic acid and related analogs exerted G1 phase antiproliferative effects in C6 glioma and limb bud cells, in a dose range of 0-3 mM. This potency did not correlate with their *in vivo* teratogenicity. However at 3mM valproic acid and related analogues caused inhibition of neuronal cell aggregation and limb bud chondrocyte differentiation in a manner that correlated with their *in vivo* teratogenicity (8).

Metabolism and toxicokinetics

Urinary excretion in humans was determined. Of the dose administered (200 mg kg⁻¹) ~40-50% was excreted in the urine within 24 hr, mainly as 5-hydroxyvalproic acid and 2-propylglutaric acid (9).

Other effects

Other adverse effects (human)

Out of 8 pregnant women who had taken valproate as an antiepileptic drug, 2 babies had facial abnormalities and 1 baby had a heart lesion (10).

Any other adverse effects

With maximally stimulating concentrations of human choriogonadotrophin or cAMP, *in vitro* testosterone formation in rats was inhibited by 50% in the presence of >1mM. With submaximally stimulating concentrations of human choriogonadotrophin, leading to physiological testosterone rates, half-maximal inhibition occurred in the presence of 900 µM (11).

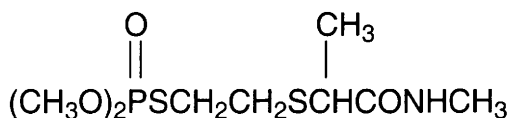
Other comments

Teratogenicity, side-effects, neurophysiology and biochemistry reviewed (12-15).

References

1. *Food Cosmet. Toxicol.* 1964, **2**, 327.
2. *Pharmacodynamic de l'Acide Dipropylacetique* 1968, 39.
3. *Sax's Dangerous Properties of Industrial Materials* 8th ed., 1989, Van Nostrand Reinhold, New York, NY, USA.
4. *Chimica Therapeutica* 1968, **3**, 430.
5. *Arzneim.-Forsch.* 1983, **33**, 1155.
6. Vorhees, C. V. *Teratology* 1987, **35**(2), 195-202.
7. Binkerd, P. E. et al *Fundam. Appl. Toxicol.* 1988, **11**(3), 485-493.
8. Bacon, C. L. et al *Toxicol. In Vitro* 1998, **12**(2), 101-109.
9. Fisher, J. E. et al *Epilepsia (N.Y.)* 1991, **32**(1), 146-150.
10. Lander, C. M. et al *Epilepsy Res.* 1990, **7**, 77-82.
11. Kuihn-Velten, W. et al *Eur. J. Pharmacol.* 1990, **181**(1-2), 151-155.
12. Lammer, E. J. et al *Teratology* 1987, **35**(3), 465-473.
13. Yamauchi, T. *Shinkei Seishin Yakuri* 1989, **11**(2), 111-119.
14. Cotariv, D. et al *Prog. Neurobiol. (Oxford)* 1990, **34**(4), 343-354.
15. Robert, E. *Congenital Anomalies* 1988, **28**(Suppl.), S71-S80

v9 vamidothion



C₈H₁₈NO₄PS₂

Mol. Wt. 287.34

CAS Registry No. 2275-23-2

Synonyms O,O-dimethyl S-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]thio]ethyl] phosphorothioate; Kilval; RP 9895; Vamidoate

EINECS No. 218-894-8

RTECS No. TF 7900000

Uses Acaricide. Insecticide.

Physical properties

M. Pt. 43°C **Volatility** v.p. negligible at 20°C

Solubility Water: 4 kg l⁻¹. Organic solvents: benzene, ethyl acetate, methyl ethyl ketone, toluene

Occupational exposure

Supply classification toxic, dangerous for the environment

Risk phrases Harmful in contact with skin – Toxic if swallowed – Very toxic to aquatic organisms (R21, R25, R50)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Wear suitable protective clothing and gloves - In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S36/37, S45, S61)

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) carp >40 mg l⁻¹ (1).

LC₅₀ (96 hr) zebra fish 590 mg l⁻¹ (2).

Invertebrate toxicity

Toxic to bees (3).

Environmental fate

Degradation studies

In soil t_{1/2} 1.0-1.5 day at 25°C. Metabolised in plants to the corresponding sulfoxide, also demethylation and hydrolysis to phosphoric acid (2).

Abiotic removal

61% removal from wastewater effected by filtration using an organic filter medium of peat and moss (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral pheasant 35 mg kg⁻¹ (2).

LD₅₀ oral mouse, rat, guinea pig, dog 40-110 mg kg⁻¹ (5-7).

LC₅₀ (4 hr) inhalation rat 1.73 g m⁻³ (3).

LD₅₀ dermal mouse 1500 mg kg⁻¹ (7).

LD₅₀ dermal rabbit 160 mg kg⁻¹ (8).

Sub-acute and sub-chronic data

Oral rat (90 day) 50 mg kg⁻¹ diet did not affect growth rate (2).

Metabolism and toxicokinetics

In vitro rat and mouse liver, it was rapidly oxidised to the sulfoxide which was the principal metabolite (9,10).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538 with and without metabolic activation positive (11).

Escherichia coli WP2 *hcr* with and without metabolic activation positive (11).

In vitro Chinese hamster ovary cells chromosomal aberrations, sister chromatid exchanges positive (metabolic activation unspecified) (12).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (13).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (14).

EEC maximum residue levels: pome fruit 0.5 ppm; other fruit and vegetables 0.05 ppm (2).

WHO Toxicity Class Ib (15).

EPA Toxicity Class II (3).

ADI (JMPR) 0.008 mg kg⁻¹ body weight (3).

References

1. Nishiucki, Y. et al *Botyu-Kagaku* 1967, **32**, 5-11.
2. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
3. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
4. Toller, G. et al *Water Res.* 1988, **22**(5), 657-661.
5. Frear, E. H. *Pesticide Index* 1976, **5**, 233, College Science Publications, State College, PA, USA.
6. *Med. Zh. Uzbek.* 1972, **8**, 65.
7. *Guide to the Chemicals Used in Crop Protection* 1973, **6**, 530, Information Canada, Ottawa, Ontario, Canada.
8. *World Rev. Pest Control* 1970, **9**, 119.
9. El-Oshar, M. A. et al *J. Agric. Food Chem.* 1987, **35**(1), 138-144.
10. El-Oshar, M. A. et al *Pestic. Biochem. Physiol.* 1987, **27**(1), 132-141.
11. Moriya, M. et al *Mutat. Res.* 1983, **116**(3/4), 185-216.
12. Taguka, H. et al *Mutat. Res.* 1980, **78**(2), 177-191.
13. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
14. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
15. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21

V10 vanadium

V

V

Mol. Wt. 50.94

CAS Registry No. 7440-62-2

EINECS No. 231-171-1

RTECS No. YW 1355000

Uses Manufacture of stainless steel.

Occurrence Widespread in nature, occurring in >65 minerals, including patronite, vanadinite, roscelite, and carnotite. Abundance in Earth's crust 0.01% by weight. Occurs in fuel oil. Released into the atmosphere from metal works and fossil fuel burning (1).

Physical properties

M. Pt. 1917°C B. Pt. 3380°C Specific gravity 6.11 at 18.7°C

Ecotoxicity

Bioaccumulation

Bioconcentration factor 50 for invertebrates, 10 for fish, 100 for aquatic plants (form unspecified) (2).

Tissue accumulation in carp was highest in the liver, then bone and muscle (form unspecified) (3).

Mammalian & avian toxicity

Acute data

LD₅₀ subcutaneous rabbit 59 mg kg⁻¹ (form unspecified) (4).

Sub-acute and sub-chronic data

Gavage rat 1 mg kg⁻¹ day⁻¹ (unspecified) for 30 days enhanced lipid peroxidation in liver and depressed other antioxidant factors (glutathione, total thiols, ascorbic acid). Vanadium decreased glutathione reductase and catalase, elevated superoxide dismutase, but had no effect on glutathione peroxidase. The authors discussed the results in terms of membrane dysfunction (5).

Irritancy

Irritating to the skin and eyes (species unspecified) (6).

Genotoxicity

Vanadium compounds were shown to induce point mutations in *Bacillus subtilis* (7).

Other effects

Other adverse effects (human)

Vanadium is a natural component of fuel oil and exposed workers have developed vanadium poisoning which is characterised by chronic respiratory effects and allergy-like eczematous skin lesions (8-10).

Any other adverse effects

In the pigeon, vanadium administration increased the secretion of thyroid hormones. The testicular tubules and interstitial cells became hypertrophied, whereas the ovaries showed follicular atresia (11).

Other comments

Vanadium has been reported to have insulin-like properties and has been demonstrated to be beneficial in the treatment of diabetic animals (12).

Biochemical role of vanadium in regulation of metabolism reviewed (13,14).

Environmental fate and toxicology reviewed (15).

Reviews on human health effects, experimental toxicology, physico-chemicals properties listed (16).

References

1. Friberg, L. et al (Eds.) *Handbook on the Toxicology of Metals* 2nd ed., 1986, 2, 2642, Elsevier, Amsterdam, Netherlands.
2. *Dangerous Prop. Ind. Mater. Rep.* 1989, 9(5), 91-96.
3. Zhang, G. et al Huangjing Wurao Yu Fangzhi 1989, 11(1), 29-31 (Ch.) (*Chem. Abstr.* 111, 2832k).
4. *Farmakol. Toksikol. (Moscow)* 1965, 28, 83.
5. Gill, K. D. et al *Med. Sci. Res.* 1988, 16(22), 1151-1152.
6. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, 2, 3591, Sigma-Aldrich, Milwaukee, WI, USA.
7. Seiler, H. G. et al (Eds.) *Handbook on the Toxicity of Inorganic Compounds* 1988, Marcel Dekker, New York, NY, USA.
8. NIOSH Criteria Document, *Vanadium* 1977, 43, DHEW Publ. NIOSH 77-222.
9. Baselt, R. C. *Biological Monitoring Methods for Industrial Chemicals* 1980, 270.
10. National Research Council *Drinking Water and Health* 1977, 1, 298, National Academy Press, Washington, DC, USA.
11. Diwan, M. et al *J. Environ. Biol.* 1987, 8(2), 157-166.
12. Ramanadham, S. et al *Can. J. Physiol. Pharmacol.* 1990, 68(4), 486-491.
13. Willsky, G. R. *Vanadium Biol. Syst.* 1990, 1-24, Klumer, Dordrecht, Netherlands.
14. Wever, R. et al *Adv. Inorg. Chem.* 1990, 38, 81-115.
15. *IPCS Environmental Health Criteria No. 81* 1988, WHO, Geneva, Switzerland.
16. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

V11 vanadium oxytrichloride



Cl₃OV

Mol. Wt. 173.30

CAS Registry No. 7727-18-6

Synonyms trichlorooxovanadium; vanadyl trichloride

EINECS No. 231-780-2

RTECS No. YW 2975000

Uses Catalyst.

Physical properties

M. Pt. -77°C B. Pt. 126-127°C Specific gravity 1.840 Volatility v.p. 13.8 mmHg at 20°C
Solubility Organic solvents: acetic acid, diethyl ether, ethanol

Occupational exposure

UN No. 2443 HAZCHEM Code 2X Conveyance classification corrosive substance

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow 13-15 mg l⁻¹ (as vanadium) (1).

Invertebrate toxicity

Yeast growth inhibition threshold 200 ppm (as vanadium) (2).

Bioaccumulation

Bioconcentration factor for mussel 2-10 (as vanadium) (3).

Environmental fate

Abiotic removal

Decomposes in cold water (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 140 mg kg⁻¹ (4).

Metabolism and toxicokinetics

Following intratracheal instillation in rats, >50% was removed from the lung within 15 min, and vanadium was transported to all organs except the brain. Bones accumulated a large proportion and testes a small proportion.

Excretion occurred via the urine and faeces. 3% of the burden remained after 63 days (5).

Cationic vanadium is poorly absorbed from the gastro-intestinal tract (6).

Other effects

Other adverse effects (human)

Extremely destructive to tissue of the mucous membranes, upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasms, inflammation and oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema. Liver and kidney damage and haematological effects may also occur (7).

Other comments

Physical properties, environmental and mammalian toxicity reviewed (8).

Decomposes in cold water.

References

1. McKee, J. E. et al *Water Quality Criteria* 2nd ed., 1963, State Water Quality Control Board, Pasadena, CA, USA.
2. Patel, B. et al *Analyst (London)* 1980, **115**(8), 1063-1068.
3. Miramend, P. et al *Mar. Biol.* 1980, **56**(4), 281-293.
4. *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 470.
5. Oberg, S. G. et al *Toxicology* 1978, **11**(4), 315-324.
6. Venugopal, B. et al *Metal Toxicity in Mammals* 1978, 211, Plenum, New York, NY, USA.
7. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3593, Sigma-Aldrich, Milwaukee, WI, USA.
8. *Dangerous Prop. Ind. Mater. Rep.* 1989, **9**(5), 91-96

V12 vanadium pentoxide



O_5V_2

Mol. Wt. 181.88

CAS Registry No. 1314-62-1

Synonyms C.I. 77938; vanadic anhydride

EINECS No. 215-239-8

RTECS No. YW 2450000

Uses Catalyst. Mordant in dyeing. In photographic developers.

Physical properties

M. Pt. 690°C B. Pt. 1750°C (decomp.) Specific gravity 3.357 at 18°C

Solubility Water: 0.8%

Occupational exposure

DE-MAK 0.05 mg m⁻³ (respirable fraction of aerosol)

FR-VME 0.05 mg m⁻³ (dust and fume) (as V₂O₅)

JP-OEL 0.1 mg m⁻³ (fume), 0.5 mg m⁻³ (dust)

SE-LEVL 0.2 mg m⁻³ (as V) (total dust) SE-CEIL 0.05 mg m⁻³ (as V) (respirable dust)

UK-LTEL 0.5 mg m⁻³ (as V) (total inhalable dust); 0.04 mg m⁻³ (as V) (fume and respirable dust)

US-TWA 0.05 mg m⁻³ (respirable dust or fume as V₂O₅)

UN No. 2862 (non-fused) HAZCHEM Code 2Z (non-fused) Conveyance classification toxic substance (non-fused)

Supply classification harmful

Risk phrases Harmful by inhalation (R20)

Safety phrases Keep out of reach of children (if sold to general public) – Do not breathe dust (S2, S22)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 10, 23 mg kg⁻¹, respectively (1,2).

LC_{Lo} (2 hr) inhalation rat 70 mg m⁻³ (3).

LD₅₀ subcutaneous rat 14 mg kg⁻¹ (1).

LD₅₀ intraperitoneal rat 12 mg kg⁻¹ (1).

Carcinogenicity and chronic effects

Intratracheal rat 0.56 mg kg⁻¹ month⁻¹ for 12 months. A reduction in body weight gain was observed following the 10th treatment. Lung weight was significantly increased. Blood glucose was slightly decreased, while blood cholesterol was markedly reduced (4).

Inhalation rabbit, rat (12 month) 10-70 mg m⁻³ 2 hr day⁻¹ caused fatty changes with partial cell necrosis in the liver. Other effects included a marked reduction in albumin/globulin ratio in serum and in liver tissue respiration (5).

Teratogenicity and reproductive effects

Intravenous mouse, lowest toxic dose 11,000 mg kg⁻¹ day⁻¹ on days 6-15 of gestation, teratogenic effects to musculoskeletal system (6).

Intraperitoneal mouse 5000 mg kg⁻¹ day⁻¹ at different times of gestation. No adverse effects were noted on pre-implantation and premature birth. However, foetotoxicity was demonstrated by increased frequency of resorption and foetal death when administered on days 6-15, 7, and 14-17 of gestation. Delayed ossification of bones was noted in the offspring of dams treated on days 6-15, 8, 10 and 14-17 of gestation (7).

Metabolism and toxicokinetics

Absorption of dust by inhalation is almost 100% in humans (8).

Irritancy

Irritating to the skin, eyes, mucous membrane and upper respiratory tract (species unspecified) (9).

Vanadium pentoxide is the only vanadium compound for which ocular disturbances have been reported (10).

Genotoxicity

In vitro human lymphocytes sister chromatid exchanges, chromosomal aberrations and polyploidy positive (11).

Other effects

Other adverse effects (human)

Dose-related increases in hyperdiploidy were seen in human lymphocyte cultures treated with 0.001-0.1 μM vanadium pentoxide. This effect may occur through a disruption of microtubule function (12).

Reported to be a respiratory irritant and to cause skin pallor, green-black tongue, chest pain, cough, dyspnoea, palpitation and lung changes. Ingestion causes gastro-intestinal disturbances (13).

Any other adverse effects

Inhibited rat liver mitochondrial respiration *in vivo* and *in vitro* (14).

Other comments

Occurs in the fly ash of oil-fired power plants (15).

Physical properties and toxicology reviewed (16).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (17).

References

1. Arch. Toxikol. 1956, **16**, 182.
2. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
3. NTIS Report AEC-TR-6710, Natl. Tech. Inf. Ser., Springfield, VA, USA.
4. Zychlinski, L. et al Arch. Environ. Contam. Toxicol. 1991, **20**(3), 295-298.
5. Friberg, L. et al *Handbook on the Toxicology of Metals* 2nd ed., 1986, **2**, 652, Elsevier, Amsterdam, Netherlands.
6. Environ. Res. 1984, **33**, 47.
7. Zang, T. et al Huaxi Yike Daxue Xuebao 1991, **22**(2), 192-195 (Ch.) (Chem. Abstr. 115, 108303h).
8. Lewis, R. J. *Sax's Dangerous Properties of Industrial Materials* 8th ed., 1992, **3**, 3479, Van Nostrand Reinhold, New York, NY, USA.
9. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3592, Sigma-Aldrich, Milwaukee, WI, USA.
10. Grant, W. M. *Toxicology of the Eye* 3rd ed., 1986, 970, Charles C Thomas, Springfield, IL, USA.
11. Rolden, R. E. et al Mutat. Res. 1990, **245**(2), 61-65.
12. Ramirez, P. et al Mutat. Res. 1997, **386**(3), 291-298.
13. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
14. Zychlinski, L. et al Arch. Environ. Contam. Toxicol. 1990, **19**(1), 138-142.
15. Schiff, L. J. et al Environ. Res. 1984, **34**(2), 390-402.
16. *Dangerous Prop. Ind. Mater. Rep.* 1988, **8**(4), 81-86.
17. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

V13 vanadium tetrachloride



Cl_4V

Mol. Wt. 192.75

CAS Registry No. 7632-51-1

Synonyms vanadium chloride

EINECS No. 231-561-1

RTECS No. YW 2625000

Uses Catalyst.

Physical properties

M. Pt. -28°C B. Pt. 154°C Specific gravity 1.816 at 30°C Volatility v.p. 5.9 mmHg at 20°C ; v.den. 6.0

Solubility Organic solvents: acetic acid, chloroform, diethyl ether, ethanol

Occupational exposure

UN No. 2444 HAZCHEM Code 4WE Conveyance classification corrosive substance

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 160 mg kg⁻¹ (1).

Carcinogenicity and chronic effects

Inhalation rat, rabbit (9-12 month) 10-70 mg kg⁻¹ 2 hr day⁻¹ caused fatty changes with partial cell necrosis in the liver. Other effects included a marked reduction in albumin/globulin ratio in serum and a drastic reduction in liver tissue respiration (2).

Other comments

Carcinogenicity and mutagenicity in hamster cells reviewed (3).

References

1. *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 470.
2. Friberg, L. et al (Eds.) *Handbook on the Toxicology of Metals* 2nd ed., 1986, **2**, 652, Elsevier, Amsterdam, Netherlands.
3. Casto, B. C. *Adv. Mod. Environ. Toxicol.* 1980, **1**(Mamm. Cell Transform. Chem. Carcinog.), 241-271

V14 vanadium trichloride



Cl_3V

Mol. Wt. 157.30

CAS Registry No. 7718-98-1

Synonyms vanadium(III) chloride

EINECS No. 231-744-6

RTECS No. YW 2800000

Uses Catalyst.

Physical properties

M. Pt. decomposes on heating Specific gravity 3.0 at 18°C

Occupational exposure

UN No. 2475 HAZCHEM Code 2X Conveyance classification corrosive substance

Mammalian & avian toxicity

Acute data

LD₃₀ oral rat 350 mg kg⁻¹ (1).

LD_{Lo} subcutaneous rabbit 20 mg kg⁻¹ (2).

Other effects

Other adverse effects (human)

Extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema (3).

References

1. *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 470.
2. *Environ. Qual. Saf. Suppl.* 1975, **1**, 1.
3. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **22**, 3592, Sigma-Aldrich, Milwaukee, WI, USA

V15 vanadium trioxide



O₃V₂

Mol. Wt. 149.88

CAS Registry No. 1314-34-7

Synonyms divanadium trioxide; vanadium(III) oxide; vanadium sesquioxide

EINECS No. 215-230-9

RTECS No. YW 3050000

Uses Catalyst.

Physical properties

M. Pt. 1940°C Specific gravity 4.870 at 18°C with respect to water at 4°C

Occupational exposure

UN No. 2860

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 130 mg kg⁻¹ (1).

LD₅₀ intratracheal rat 125 mg kg⁻¹ (2).

Carcinogenicity and chronic effects

Inhalation rabbit (12 month) 10-75 mg m⁻³ 2 hr day⁻¹ caused sneezing, nasal discharge, dyspnoea, tachypnoea, and in some cases bronchial asthma. Fatty changes with partial cell necrosis in the liver, a marked reduction in albumin/globulin ratio in serum, and reduction in liver tissue respiration were also reported (3).

Metabolism and toxicokinetics

Following exposure of humans to vanadium trioxide dust, the greatest amount of vanadium was found in the urine 3 days after exposure. None was detectable after 1 wk. None was detectable in faeces after 2 wk (4).

Irritancy

Irritating the skin, eyes, mucous membranes and upper respiratory tract (species unspecified) (5).

Genotoxicity

In vitro Chinese hamster ovary cells with metabolic activation sister chromatid exchanges positive (6).

In vitro human fibroblasts chromosomal aberrations positive (7).

References

1. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals under Single Exposure* 1982, CIP, Moscow, USSR.
2. *NTIS Report EAC-TR-6710*, Natl. Tech. Inf. Ser., Springfield, VA, USA.
3. Friberg, L. et al (Eds.) *Handbook on the Toxicology of Metals* 2nd ed., 1986, 2, 648, Elsevier, Amsterdam, Netherlands.
4. National Research Council *Drinking Water and Health* 1977, 1, 297, National Academy Press, Washington, DC, USA.
5. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, 2, 3592, Sigma-Aldrich, Milwaukee, WI, USA.
6. Owusu-Yaw, J. et al *Toxicol. Lett.* 1990, 50(2-3), 327-336.
7. Seiler, H. G. et al (Eds.) *Handbook on Toxicity of Inorganic Compounds* 1988, 753, Marcel Dekker, New York, NY, USA

V16 vanadyl sulfate



O₅SV

Mol. Wt. 163.00

CAS Registry No. 27774-13-6

Synonyms C.I. 77940; oxo[sulfato(2-)-O]vanadium; oxysulfatovanadium; vanadium oxysulfate

EINECS No. 248-652-7

RTECS No. YW 1925000

Uses Catalyst. Mordant in dyeing. Pigment in ceramics.

Occurrence In fly ash of oil-fired power plant (1).

Physical properties

Solubility Water: freely soluble (dihydrate)

Occupational exposure

UN No. 2931 HAZCHEM Code 2Z Conveyance classification toxic substance

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bluegill sunfish 6-55 mg l⁻¹ (2).

LC₅₀ (7 day) goldfish 3.0 mg l⁻¹ (as vanadium) (3).

Mammalian & avian toxicity

Acute data

LD₅₀ subcutaneous mouse 560 mg kg⁻¹ (4).

LD₅₀ intraperitoneal mouse 140 mg kg⁻¹ (5).

Sub-acute and sub-chronic data

Gavage rat 0.5 LD₅₀ 6 × wk⁻¹ for 2-12 wk caused a decrease in calcium and phosphorus content and alkaline phosphatase activity in the bones. Vanadium content of the bones was increased (6).
Oral rat 3.75 mg kg⁻¹ as vanadium 6 × wk⁻¹ for 42 wk decreased calcium absorption in the duodenum by 30%. A 37% decrease was observed 4-6 wk following a single oral dose of 15 mg kg⁻¹ as vanadium (7).
Oral rat (3 month) 5 ppm in drinking water caused no significant effect on body weight or haematocrit values (8).
Oral rabbit (6 wk) 500 ppm diet mobilised excess arterial cholesterol in animals previously maintained on a cholesterol-rich diet (9).

Sensitisation

5% solution has a sensitising effect on guinea pig skin (9).

Genotoxicity

Saccharomyces cerevisiae increased mitotic recombination frequency (10).
In vitro Chinese hamster ovary cells with and without metabolic activation sister chromatid exchanges positive (11).

Other effects

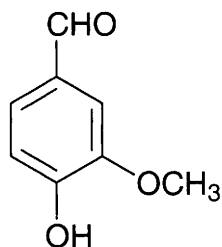
Any other adverse effects

Intraperitoneal rats (3 day) 0.63 mg V kg⁻¹ day⁻¹ (as NaVO₃ or VOSO₄). Vanadium accumulated in liver nuclei exclusively in the vanadyl sulfate (4+ oxidation state). Incubation of DNA with vanadyl ions and hydrogen peroxide led to intense DNA cleavage, suggesting that the mechanism for vanadium dependent toxicity and antineoplastic action is due to DNA cleavage by hydroxyl radicals generated in living systems (12).

References

1. Schiff, L. J. et al *Environ. Res.* 1984, **34**(2), 390-402.
2. Tarzwell, C. M. et al *Ind. Wastes* 1960, **5**, 12.
3. Knudtson, B. K. *Bull. Environ. Contam. Toxicol.* 1979, **23**, 95-99.
4. *Russ. Pharmacol. Toxicol.* 1971, **34**(3), 135.
5. *C. R. Acad. Sci.* 1963, **256**, 1043.
6. Witkowska, D. et al *Bromatol. Chem. Toksykol.* 1986, **19**(4), 258-263 (Pol.) (*Chem. Abstr.* **107**, 2246m).
7. Witkowska, D. et al *Bull. Environ. Contam. Toxicol.* 1986, **37**(6), 899-906.
8. Parker, R. et al *J. Environ. Pathol. Toxicol.* 1978, **2**(2), 235-246.
9. Friberg, L. et al (Eds.) *Handbook on the Toxicology of Metals* 2nd ed., 1986, **2**, 644, Elsevier, Amsterdam, Netherlands.
10. Sora, S. et al *Mutagenesis* 1986, **1**(1), 21-28.
11. Owusu-Yaw, J. et al *Toxicol. Lett.* 1990, **50**(2-3), 327-336.
12. Sakurai, H. *Environ. Health Perspect.* 1994, **102**(Suppl. 3), 35-36

V17 vanillin



$C_8H_8O_3$

Mol. Wt. 152.15

CAS Registry No. 121-33-5

Synonyms FEMA No. 3107; 4-hydroxy-*m*-anisaldehyde; 4-hydroxy-3-methoxybenzaldehyde; bioxin; 3-methoxy-4-hydroxybenzaldehyde; methyl protocatechuic aldehyde; vanilla; vanillaldehyde; vanillic aldehyde; *p*-vanillin; Zimco

EINECS No. 204-465-2

RTECS No. YW 5775000

Uses Organic synthesis. In deodorants. Flavour agent in confectionery and cosmetics. Analytical reagent. Insect attractant.

Occurrence Extracted from vanilla. In potato parings, Siam benzoin, etc. (1).

Physical properties

M. Pt. 81-83°C **B. Pt.** 285°C **Specific gravity** 1.056 **Partition coefficient** $\log P_{ow}$ 1.26 (2)

Volatility v.p. 1 mmHg at 107°C ; v.den. 5.2

Solubility Water: 1% at 20°C. Organic solvents: acetone, chloroform, diethyl ether, ethanol, pyridine

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow 120 mg l⁻¹ – static bioassay (3).

Environmental fate

Degradation studies

Utilised as sole carbon source by *Bacillus subtilis* (4).

Abiotic removal

Adsorbed by activated carbon with micropores of radius <1.5-1.6 × 10⁻⁶ mm (5).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, guinea pig 1400, 1600 mg kg⁻¹, respectively (6).

LD₅₀ subcutaneous rat 1500 mg kg⁻¹ (7).

LD₅₀ intraperitoneal rat, mouse, guinea pig 480, 1200, 1160 mg kg⁻¹, respectively (8,9).

Carcinogenicity and chronic effects

Oral rat (2 yr) 5000, 10,000 or 20,000 ppm diet caused no adverse effects (10).

Teratogenicity and reproductive effects

Subcutaneous ♀ rat, lowest toxic dose 20 mg kg⁻¹ 4 days prior to mating – effects to ovaries, fallopian tube, uterus and cervix (11).

Metabolism and toxicokinetics

Urinary metabolites identified following intraperitoneal administration to rats are principally vanillic acid (both free and conjugated), conjugated vanillin and vanillyl alcohol, and catechol (10).

Sensitisation

Positive in patch tests in 8/142 sensitised subjects (10).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1538 with and without metabolic activation negative (12).

In vitro human lymphocytes sister chromatid exchanges positive (1).

Legislation

ADI human 10 mg kg⁻¹ (13).

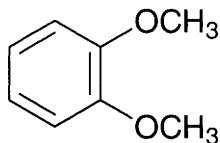
Other comments

Suppressed chromosomal aberrations in Chinese hamster cells induced by UV light or X-rays *in vitro* and decreased the *in vivo* ethylnitrosourea-induced frequency of recessive carrier in rat pups (14,15).

References

1. Jansson, T. et al *Mutat. Res.* 1986, **169**, 129-139.
2. Bodor, N. et al *J. Am. Chem. Sci.* 1989, **111**(11), 3783-3786.
3. Mattson, V. R. et al *Acute Toxicity of Selected Organic Chemicals to Fathead Minnows* 1976, US EPA, EPA-600/3-76-097.
4. Gurujeyalakshmi, G. *Curr. Microbiol.* 1987, **16**(2), 69-73.
5. Tenada, S. et al *Igaku to Seibutsugaku* 1987, **114**(4), 263-265 (Japan.) (*Chem. Abstr.* **107**, 140422s).
6. Jenner, P. M. et al *Food Cosmet. Toxicol.* 1964, **2**, 327.
7. *Rev. Med. Suisse Romand.* 1896, **16**, 449.
8. *FAO Report Series* 1967, **44A**, 79, WHO, Washington, DC, USA.
9. *C. R. Acad. Sci.* 1956, **243**, 609.
10. *Patty's Industrial Hygiene and Toxicology* 3rd ed., 1981 **2A**, 2539-2541, Wiley Interscience, New York, NY, USA.
11. *J. Sci. Ind. Res. Biol. Sci.* 1960, **19**, 264.
12. Mortelmans, K. et al *Environ. Mutagen.* 1986, **8**(Suppl. 7), 1-119.
13. *Summary of Evaluations Performed by the Joint FAO/WHO Expert Committee on Food Additives (JECFA)* 1996, International Programme on Chemical Safety, WHO, Geneva, Switzerland.
14. Sasaki, Y. F. et al *Mutat. Res.* 1990, **229**(1), 1-10.
15. Imanishi, H. et al *Mutat. Res.* 1990, **243**(2), 151-158

V18 veratrole



$C_8H_{10}O_2$

Mol. Wt. 138.17

CAS Registry No. 91-16-7

Synonyms catechol dimethyl ether; *o*-dimethoxybenzene; 1,2-dimethoxybenzene; *O,O*-dimethylcatechol; *O*-hydroquinine dimethyl ether; 2-methoxyanisole; pyrocatechol dimethyl ether

EINECS No. 202-045-3

RTECS No. CZ 6475000

Uses Organic synthesis. Weathering agent in paints and plastics. Flavouring. Manufacture of dyestuffs. In cosmetics.

Occurrence In essential oils of *Hyacinthus orientalis* and *Rhodophyllus icterus*

Physical properties

M. Pt. 22-23°C **B. Pt.** 206-207°C **Flash point** 87°C **Specific gravity** 1.084 at 25°C with respect to water at 25°C

Solubility Water: miscible. Organic solvents: acetone, benzene, diethyl ether, ethanol, olive oil

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow 120 mg kg⁻¹ flow-through bioassay (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 700, 2000 mg kg⁻¹, respectively (2,3).

Sub-acute and sub-chronic data

Oral rat, 0.5 or 2% diet for 7 wk depressed growth rate in a dose-dependent manner (4).

Irritancy

Dermal guinea pig (24 hr) 40% solution in olive oil and instillation into guinea pig eye for 24 hr caused slight to moderate irritation (5).

References

1. Veith, G. D. et al *Can. J. Fish. Aquat. Sci.* 1983, **40**(6), 743-748.
2. *Gig. Tr. Prof. Zabol.* 1982, **26**(2), 54.
3. Jenner, P. M. et al *Food Cosmet. Toxicol.* 1964, **2**, 327.
4. Hodge, H. C. et al *J. Ind. Hyg. Toxicol.* 1949, **31**, 79.
5. *Patty's Industrial Hygiene and Toxicology* 3rd ed., 1981, **29**, 2527, Interscience Publishers, New York, NY, USA

V19 vernolate



$\text{C}_{10}\text{H}_{21}\text{NOS}$

Mol. Wt. 203.35

CAS Registry No. 1929-77-7

Synonyms S-propyl dipropylthiocarbamate; S-propyl carbamothioate; PPTC; R-1607; Reward; Saverit; Savirox; Vernam

EINECS No. 217-681-7

RTECS No. FA 4725000

Uses Herbicide.

Physical properties

B. Pt. 150°C at 30 mmHg **Flash point** 121°C **Specific gravity** 0.952 at 20°C with respect to water at 20°C

Partition coefficient $\log P_{\text{ow}}$ 3.844 at 20°C (1) **Volatility** v.p. 1.0×10^{-5} mmHg at 25°C

Solubility Water: 90 mg l⁻¹ at 20°C. Organic solvents: diethyl ether, ethanol, methyl isobutyl ketone, kerosene, xylene

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed (R22)

Safety phrases Keep out of reach of children (if sold to general public) (S2)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bluegill sunfish, rainbow trout 8.4, 9.6 mg l⁻¹, respectively (1).

Invertebrate toxicity

LC₅₀ (96 hr) *Gammarus lacustris*, *Gammarus fasciatus* 1.8-13 mg l⁻¹ (2,3).

LC₅₀ (48 hr) *Daphnia magna*, *Cypridopsis vidua*, *Asellus cranicardus*, *Palaemonetes kadiakersis*, *Orconectes nais* 1.1-24 mg l⁻¹ (3).

Non-toxic to bees at 0.11 mg bee⁻¹ (4).

Environmental fate

Degradation studies

In soil undergoes microbial degradation to mercaptan, amine, carbon dioxide and isopropanol. $t_{1/2}$ 8-16 days at 27°C, >64 days at 4°C (1).

Degraded by *Streptomyces*, *Mycobacterium* and *Flavobacterium* sp. (5).

Abiotic removal

Decomposed by sunlight (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird, starling >100 mg kg⁻¹ (6).

LD₅₀ oral rat 1200-1800 mg kg⁻¹ (1,7,8).

LD₅₀ dermal rabbit >5000 mg kg⁻¹ (1).

LC₅₀ (4 hr) inhalation rat >5 mg l⁻¹ (4).

Sub-acute and sub-chronic data

LC₅₀ (7 day) oral bobwhite quail 12,000 mg kg⁻¹ diet (1).

Oral rat, dog (90 day) no-adverse effect level 32-38 mg kg⁻¹ day⁻¹ (1).

Irritancy

Non-irritating to rabbit eye and skin (1).

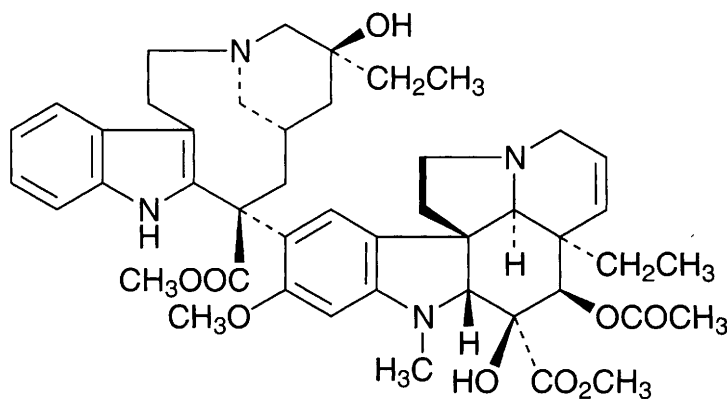
Legislation

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (9).
Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (10).
Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (11).
WHO Toxicity Class II (12).
EPA Toxicity Class III (formulation) (4).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. Sanders, H. O. *Toxicity of Pesticides to the Crustacean, Gammarus lacustris* 1969, Bureau Sport Fisheries and Wildlife, Technical Paper 25, Washington, DC, USA.
3. Sanders, H. O. *J. Water Pollut. Control Fed.* 1970, **42**(8, Part 1), 1544-1550.
4. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
5. Imai, Y. et al *Nipon Nayaku Gakkaishi* 1986, **11**(4), 563-572.
6. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
7. Bailey, G. W. et al *Res. Rev.* 1965, **10**, 97.
8. *Farm Chemicals Handbook* 1983, C252, Meister, Willoughby, OH, USA.
9. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
10. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
11. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
12. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21

v20 vinblastine



$\text{C}_{46}\text{H}_{58}\text{N}_4\text{O}_9$

Mol. Wt. 810.99

CAS Registry No. 865-21-4

Synonyms Vincal leukoblastine; VLB; 29060-LE

EINECS No. 212-734-0

RTECS No. YY 8050000

Uses Antineoplastic agent.

Occurrence Alkaloid isolated from several members of the plant genus *Cathoreanthus* (formerly called *Vinca*) (1).

Physical properties

M. Pt. 211-216°C

Solubility Water: Practically insoluble. Organic solvents: acetone, alcohols, chloroform, ethyl acetate

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal mouse 7.3 mg kg⁻¹ (2).

Teratogenicity and reproductive effects

Intraperitoneal rat 0.12-0.50 mg kg⁻¹ day⁻¹ on days 7-12 of gestation. Embryo lethality was 20% in the low-dose, to 80% in the high-dose group. Malformations occurred in 9.4% of foetuses that survived the maternal dose of 0.25 mg kg⁻¹, and 2.6 % (2/78) of the foetuses of the low-dose group. The abnormalities observed included exencephaly, rachischisis and gastroschisis (3).

Intravenous rat 1 mg animal⁻¹ on day 15 of gestation. The number of mitotic figures 1000 cells⁻¹ after 4 hr increased 6.5-fold in maternal bone marrow, 5.7-fold in foetal cell suspensions, but only 1.7-fold in a placental cell suspension (4).

Administration of 0.1-0.5 LD₅₀ (route unspecified) to mice included testicular cytotoxicity, as determined by testicular weight, the repopulation index and histology (5).

Metabolism and toxicokinetics

24 hr after intravenous injection of tritiated vinblastine to rats, radioactivity was distributed evenly throughout the body. At that time <7% of total injected radioactivity was excreted in the urine. There was evidence of biliary excretion, and 2 hr after injection the lung, liver, spleen and kidney contained the highest concentrations (6,7).

Genotoxicity

In vitro mouse bone marrow cells and human lymphocytes micronuclei formation and sperm abnormalities positive. Since vinblastine produces changes in mitotic spindle formation, whether these changes are related to mutagenicity is questionable (1,8,9).

In vivo mouse bone marrow induction of aneuploidy and polyploidy positive (10).

Hexaploid wheat assay, induction of aneuploidy positive (11).

Other effects

Other adverse effects (human)

Not toxic to human erythrocytes *in vitro* (12).

Any other adverse effects

Intraperitoneal mouse, single doses of 1.5 or 5.0 mg kg⁻¹ acted as an immunosuppressive agent on the primary cell-mediated immunity when administered after, but not before, allotransplantation antigen (2).

Inhibited protein synthesis in rat liver *in vitro* (13).

Neurotoxicity was demonstrated by selective damage to the granule cells following injection into the dentate gyrus (species unspecified) (14).

Other comments

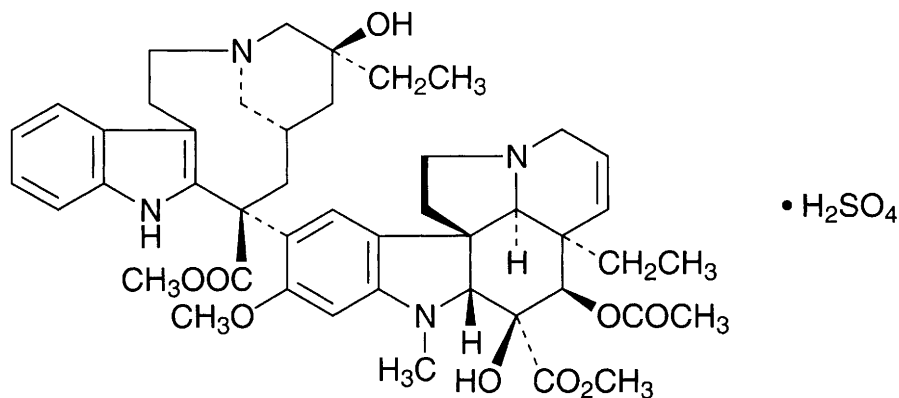
Physical properties, uses, occurrence, analysis, carcinogenicity, mammalian toxicity, metabolism and mutagenicity reviewed (1).

References

1. IARC Monograph 1981, **26**, 349-363.
2. Pyo, M. Y. *Saengyok Hakhoechi* 1986, **17**(3), 248-254 (Korean) (*Chem. Abstr.* **106**, 131406s).
3. Cohlman, S. Q. et al *J. Pediatr.* 1965, **66**, 541-544.
4. Cohlman, S.Q. et al *Lancet* 1964, **i**, 1390.
5. Kim, S. W. et al *K'at'ollik Taehah Chihakpu Nonmuryip* 1989, **42**(3), 723-733 (Korean) (*Chem. Abstr.* **112**, 111642m).

6. Beer, C. T. et al *Lloydia* 1964, **27**, 352-360.
7. Beer, C. T. et al *Can. J. Physiol. Pharmacol.* 1964, **42**, 368-373.
8. Heddle, J. A. et al *Progress in Genetic Toxicology* Scott, D. et al (Eds.) 1977, **2**, 265-274, Elsevier, Amsterdam, Netherlands.
9. Miglio, L. et al *Toxicol. In Vitro* 1991, **5**(4), 325-336.
10. Gustavino, B. et al *Mutat. Res.* 1991, **248**(1), 45-50.
11. Sandhu, S. S. et al *Mutagenesis* 1991, **6**(5), 369-373.
12. Sharma, Y. C. et al *Indian J. Cancer Chemotherap.* 1989, **11**(2), 63-66.
13. Goethals, F. et al *Toxicol. In Vitro* 1990, **4**(4-5), 435-438.
14. Goldschmidt, R. B. et al *Brain Res.* 1989, **486**(1), 133-140

v21 vinblastine sulfate



C₄₆H₆₀N₄O₁₃S

Mol. Wt. 909.07

CAS Registry No. 143-67-9

Synonyms Exal; LE 29060; NSC-49842; Velban; Velbe; vincalucoblastine sulfate (1:1); vincalucoblastine sulfate; VLB sulfate

EINECS No. 205-606-0

RTECS No. YY 8400000

Uses Antineoplastic agent, almost always used in combination with other agents (1).

Occurrence Vinblastine is isolated from several members of the plant genus *Catharanthus* (formerly called *Vinca*) (1).

Physical properties

M. Pt. 284-285°C (decomp.) (sulfate hydrate)

Solubility Water: 10%. Organic solvents: chloroform, ethanol, methanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 15 mg kg⁻¹ (2).

LD₅₀ intraperitoneal rat, mouse 2.2, 5.6 mg kg⁻¹, respectively (2).

LD₅₀ intravenous rat, mouse 2.9, 9.5 mg kg⁻¹, respectively (2,3).

In rats, the prominent signs of toxicity were diarrhoea, anorexia, locomotor inactivity, diuresis, weight loss and dyspnoea. Deaths usually occurred 3-7 days after dosing (4).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (5).

Intraperitoneal mouse (18 month) 0.09 or 0.18 mg kg⁻¹ 3 × wk⁻¹ for 6 months. The survival time of ♂ was 42% of controls and of ♀ 74-98% of controls. Tumour incidences of 1/19 ♂ mice and 4/14 ♀ mice were not significantly different from the 26% incidence among controls (6).

Intraperitoneal rat (18 month) 0.1 or 0.2 mg kg⁻¹ 3 × wk⁻¹ for 6 months. Survival time ranged from 18-100% of that of controls. Of treated ♂ rats, 11/21 had neoplasms, 7 of which were malignant (2 lymphosarcomas, 2 pituitary tumours, 1 peritoneal sarcoma, 1 reticulum-cell sarcoma, 1 testicular neoplasm). Among ♂ controls, 34% had tumours, mostly in the endocrine tissues, including pituitary, adrenal, thyroid, testes and mammary glands. Of treated ♀ rats, 18/25 had neoplasms, 3 of which were malignant; the principal sites of tumour development were the breast (11 tumours) and pituitary (7 tumours). Tumours were seen at the same sites in controls in which 58% incidence of tumours occurred (6).

Intravenous rat (2 yr) 0.14 mg kg⁻¹ wk⁻¹ for 52 wk, or 0.33 mg kg⁻¹ every 14 days for a total of 5 injections. In the first group 25/48 rats were still alive at the time of appearance of the first tumour, and only 1 rat died with a neoplasm (a benign thymoma) 18 months after the start of the experiment. In the second group 31/96 animals were still alive at the time of appearance of the first tumour; a 3% incidence of malignant tumours and 9% incidence of benign tumours were seen. Of controls, 65/89 survived to the time of the first tumour, and 5% died with benign tumours and 6% with malignancies after a median latent period of 23 months (7).

Teratogenicity and reproductive effects

Single injection of 0.3 or 0.35 mg kg⁻¹ to mice (route unspecified) on day 9 of gestation. In the high-dose group, 69% of foetuses were resorbed, and 35/74 surviving foetuses showed morphological defects such as anophthalmia, gastroschisis, umbilical hernia and twisted hind limbs. 10/74 foetuses were growth retarded. In the lower-dose group, the rate of resorption was similar at 52% but only 3/55 surviving foetuses showed malformations. Resorption rate was 5% among controls (8).

Intramuscular Long Evans or Holtzman rats, 0.025 mg on day 8 of gestation produced 51% and 33% resorption in the 2 strains, respectively. 66/143 surviving Long Evans foetuses, and 43/102 surviving Holtzman foetuses showed malformations, such as anophthalmia, microphthalmia, microcephaly or micrognathia (9).

Intraperitoneal rat 1.0 mg kg⁻¹ on day 14 of gestation. Ultrastructural changes were observed 6 hr later in the primitive neural cells of the telencephalic wall of the foetuses. The changes included abnormal accumulation of mitotic cells in metaphase on the paraventricular surface, condensation and fragmentation of chromatin materials in some cells and a decrease in complete disappearance of endoplasmic reticulum in Golgi apparatus. The changes were transient and after 9 hr only occasional necrotic cells could be seen (10).

An infant whose mother received combination therapy consisting of nitrogen mustard, procarbazine and vinblastine sulfate during the first trimester had only four toes on each foot with syndactyly of the third and fourth right toes. The fourth metatarsal was absent in the left toe (11).

Metabolism and toxicokinetics

In dogs (route unspecified), plasma levels of tritiated vinblastine sulfate fell in a biphasic mode with t_{1/2} of 17-38 min and 3-5 hr, respectively. Unchanged vinblastine was a major component of bile radioactivity. Over a 9 day period 12-17% of administered radioactivity was excreted in the urine and 30-36% in the bile (12).

In humans (route unspecified), a triphasic decay, with t_{1/2} 3.9, 53 and 1173 minutes, respectively, was identified. Using ring-tritiated substance, ~10% administered radioactivity was found in the faeces and 14% in the urine; the majority was unaccounted for. One cytotoxic metabolite, deacetyl vinblastine, was identified (13).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535, TA1538 with and without metabolic activation negative (14,15).

In vitro Chinese hamster lung cells chromosomal aberrations positive (metabolic activation unspecified) (16).

In vivo mouse dominant lethal assay negative (17).

Hexaploid wheat, induction of aneuploidy positive (18).

Other effects

Other adverse effects (human)

The dominant effect is leucopenia, which limits the therapeutic dose that can be given. High doses cause peripheral neuropathy, constipation and ileus. Alopecia, inappropriate antidiuretic hormone secretion, vocal chord paralysis and laryngeal nerve paralysis have also been reported. The majority of these effects are reversible when the drug is discontinued. Raynaud's phenomenon has also been reported as a possible complication of vinblastine therapy (1).

No birth defects were reported in four cases where vinblastine sulfate was administered during pregnancy (1). Vinblastine sulfate, mainly in combination therapy, has been associated in case reports with the subsequent development of leukaemias. The only epidemiological study reported was small and of short duration and showed no excess of subsequent neoplasms in patients treated with a regimen including vinblastine sulfate, adriamycin, bleomycin and dacarbazine (1).

In a large systematic follow-up of patients with Hodgkin's disease treated with an intensive chemotherapeutic combination including vinblastine sulfate, adriamycin, bleomycin and dacarbazine, but no alkylating agent, preliminary evidence suggested no excess of acute nonlymphocytic leukaemia in the first decade after therapy (19,20).

Other comments

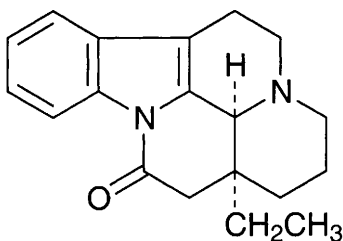
Physical properties, uses, occurrence, analysis, carcinogenicity, mammalian toxicity, metabolism and mutagenicity reviewed (1).

A distinctive feature of the vinca alkaloids is their ability to arrest cell division in the metaphase by a direct effect on the spindle apparatus. In the absence of a complete spindle, the chromosome may be dispersed through the cytoplasm or may adopt various unusual groupings. Other microtubular structures may also be affected (21).

References

1. IARC Monograph 1981, **26**, 349-363.
2. Nemeth, L. et al *Neoplasma* 1970, **17**, 345-347.
3. Sax, N. I. et al *Dangerous Properties of Industrial Materials* 8th. ed., 1992, Van Nostrand Reinhold, New York, NY, USA.
4. Todd, G. C. et al *J. Toxicol. Environ. Health* 1976, **1**, 843-850.
5. IARC Monograph 1987, **Suppl. 7**, 372.
6. Weisburger, E. K. *Cancer* 1977, **40**, 1935-1949.
7. Schmaehl, D. et al *Arzneim.-Forsch.* 1970, **20**, 1461-1467.
8. Joneja, M. G. et al *Toxicol. Appl. Pharmacol.* 1974, **27**, 408-414.
9. De Myer, W. *Neurology* 1964, **14**, 806-808.
10. Takeuchi, I. K. et al *Br. J. Exp. Pathol.* 1977, **38**, 521-532.
11. Garret, M.J. *Ann. Interim. Med.* 1974, **70**, 343-348.
12. Greasey, W. A. et al *Cancer Res.* 1975, **35**, 1116-1120.
13. Owellen, R. J. et al *Cancer Res.* 1977, **37**, 2597-2602.
14. Seino, Y. et al *Cancer Res.* 1978, **38**, 2148-2156.
15. Heddle, J. A. et al in Scott, D. et al (Eds.) *Progress in Genetic Toxicology* 1977, **2**, 265-274, Elsevier, Amsterdam, Netherlands.
16. Segawa, M. et al *Mutat. Res.* 1979, **66**, 99-102.
17. Epstein, S. S. et al *Toxicol. Appl. Pharmacol.* 1972, **23**, 288-325.
18. Redei, G. P. et al *Mutat. Res.* 1988, **201**(2), 337-348.
19. Santoro, A. et al *Cancer Treat. Rep.* 1986, **70**, 343-348.
20. Valagussa, P. et al *Blood* 1982, **59**, 488-494.
21. Greasey, W. A. et al in Sartorelli, A. C. et al (Eds.) *Antineoplastic and Immunosuppressive Agents* 1975, **Part II**, 670-694, Springer, New York, NY, USA

v22 vinburnine



$C_{19}H_{22}N_2O$

Mol. Wt. 294.40

CAS Registry No. 4880-88-0

Synonyms 1-eburnamonine; (3 α ,16 α)-eburnamenin-14(15*H*)-one; Ebernal; Ebernal Ritardo; (-)-eburnamonine; L-eburnamonine; vincamone

EINECS No. 225-490-5

RTECS No. YY 8575570

Uses Used in conditions associated with cerebral circulatory insufficiency.

Occurrence Alkaloid obtained from *Vinca minor*.

Physical properties

M. Pt. 174-177°C

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse >2000 mg kg⁻¹ (1).

LD₅₀ intraperitoneal mouse 270 mg kg⁻¹ (1).

LD₅₀ intravenous mouse 28 mg kg⁻¹ (1).

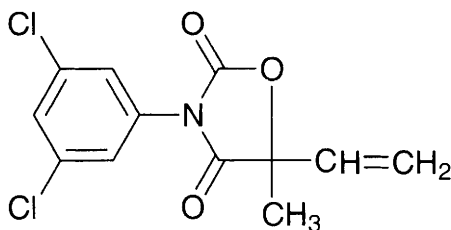
Other comments

Intraperitoneal mouse, doses up to 20 mg kg⁻¹ caused a dose-related reduction in learning and memory impairments induced by scopolamine and pentylenetetrazole (2).

References

1. *Med. Actual.* 1978, **14**, 160.
2. Drago, F. et al *Pharmacol., Biochem. Behav.* 1990, **37**(1), 53-57

v23 vinclozolin



C₁₂H₉Cl₂NO₃

Mol. Wt. 286.11

CAS Registry No. 50471-44-8

Synonyms (RS)-3-(3,5-dichlorophenyl)-5-methyl-5-vinyl-1,3-oxazolidine-2,4-dione; 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl-2,4-oxazolidinedione; Ornalin; Ronilan; Vorlan; Monitox; Pinulin; Virem; Curalan

EINECS No. 256-599-6

RTECS No. RP 8530000

Uses Fungicide.

Physical properties

M. Pt. 108°C (technical) **B. Pt.** 131°C at 0.05 mmHg **Specific gravity** 1.51 **Partition coefficient** log P_{ow} 3.00

(1) **Volatility** v.p. 1.2×10^{-7} mmHg at 20°C

Solubility Water: 3.4 mg l⁻¹ at 20°C. Organic solvents: acetone, benzene, chloroform, cyclohexane, cyclohexanone, diethyl ether, ethanol, xylene

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) guppy, trout 53, 130 mg l⁻¹, respectively (1).

Invertebrate toxicity

Not toxic to bees. LD₅₀ >250 mg bee⁻¹ (2).

Environmental fate

Degradation studies

90% degradation in soils previously treated ≥ 3 times with vinclozolin in 4-15 days, or 5-23 days in soils previously treated only once, or 22-93 days in soils previously untreated (3).

Following application of vinclozolin at the recommended maximum rate to grape vines growing in a strongly calcareous sandy loam with low organic content, rapid degradation of vinclozolin (> 98% degradation in 10 days) occurred in the soil (4).

Vinclozolin added to vineyard soil underwent 90% degradation in 7 days (5).

Abiotic removal

Undergoes hydrolysis at pH 5-9 giving 3 products identified as: 2-[[[(3,5-dichlorophenyl)carbamoyl]oxy]-2-methyl-3-butenic acid; 3',5'-dichloro-2-hydroxy-2-methylbut-3-enanilide and 3,5-dichloroaniline (6).

Vinclozolin undergoes photolytic reactions in the presence of organic and inorganic soil constituents. Humic and fulvic acids in aqueous solution lead to enhanced photo degradation of these chemicals. Iron oxide and TiO₂ contribute to the disappearance of the dicarboximide fungicides due to photocatalysis. Photolysis of these compounds leads to dechlorination and isomerisation (7).

Adsorption and retention

No leaching of vinclozolin occurred from strongly alkaline calcareous sandy loam with low organic content (1-2%) following application of vinclozolin at the maximum recommended rates to grape vines. Only very low concentrations of vinclozolin (0.05-1.4% of applied dose) were found throughout the soil core profiles, suggesting that it was mobile but also unstable in the soil (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat >10,000 mg kg⁻¹ (1).

LD₅₀ oral guinea pig 8000-10,000 mg kg⁻¹ (8,9).

LC₅₀ (4 hr) inhalation rat >29,000 mg m⁻³ (1).

LD₅₀ dermal rat >2500 mg kg⁻¹ (1).

Intraperitoneal ♂ rat, single dose of 110 or 280 mg kg⁻¹ showed no significant nephrotoxic potential (10).

Sub-acute and sub-chronic data

Oral rat, dog (90 day) no-adverse-effect level 300 mg kg⁻¹ diet for dogs, 450 mg kg⁻¹ diet for rats (1).

Carcinogenicity and chronic effects

EPA Weight-of-the-evidence category group E – evidence for noncarcinogenicity for humans (11).

Teratogenicity and reproductive effects

Vinclozolin administered orally to pregnant rats at 100 and 200 mg kg⁻¹ day⁻¹ during the period of foetal sex differentiation (gestational day 14 to post-natal day 3) induced a number of reproductive abnormalities in ♂ pups including hypospadias, cleft phallus, testicular granuloma and atrophic seminal vesicles. The evidence indicated that the developmental toxicity was mediated by antiandrogenic metabolites of vinclozolin. The authors were of the opinion that similar effects in humans are likely to occur if exposure of the foetus during sex differentiation results in similar tissue levels of metabolites (12,13).

Metabolism and toxicokinetics

Following oral administration to rats, eliminated in approximately equal proportions in the urine and faeces. The principal metabolite is *N*-(3,5-dichlorophenyl)-2-methyl-2,3,4-trihydroxybutanamide (1).

In hens, the major routes of metabolism are epoxidation of the vinyl group, followed by hydration of the intermediate epoxide, and by hydrolytic cleavage of the heterocyclic ring (14).

Genotoxicity

Salmonella typhimurium TA100 with metabolic activation positive (15).

Schizosaccharomyces pombe with metabolic activation positive (15).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (16).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (17).

EEC maximum residue limits: strawberries 15 ppm; grapes, kiwi fruit, stone fruit 10 ppm; salads 5 ppm; beans 1 ppm (1).

The log P_{ow} value exceeds the European Community recommended level of 3.0 (6th and 7th amendments) (18).

ADI (JMPR) 0.01 mg kg⁻¹ (2).

WHO Toxicity class Table 5 (19).

EPA Toxicity class IV (formulation) (2).

Other comments

Attributed endocrine disruption effects in wildlife. Avian reproduction impaired, reduced egg production, reduced fertility, impaired testicular development (20).

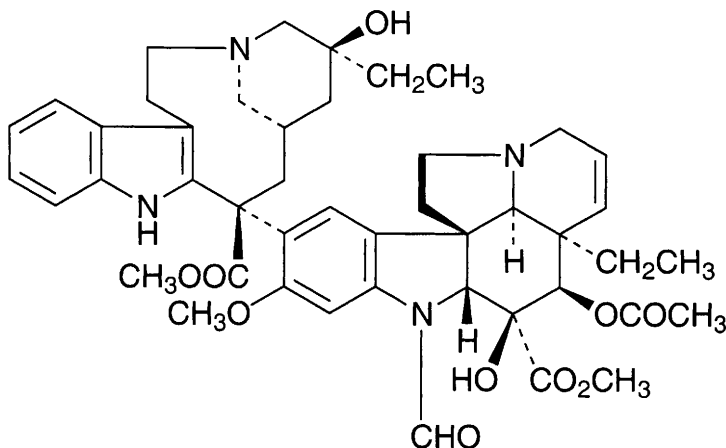
In plants, the primary metabolites are (1-carboxy-1-methyl)allyl 3,5-dichlorophenylcarbamate and *N*-(3,5-dichlorophenyl)-2-hydroxy-2-methyl-3-butenamide. Alkaline hydrolysis leads to the splitting off of 3,5-dichloroaniline. The metabolites exist as conjugates (1).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.

3. Walker, A. *Pestic. Sci.* 1987, **21**(3), 219-231.
4. Ueoka, M. et al *Chemosphere* 1997, **35**(12), 2915-2924.
5. Garcia-Cazorla, J. et al *J. Agric. Food Chem.* 1998, **46**(7), 2845-2850.
6. Szeto, S. Y. et al *J. Agric. Food Chem.* 1989, **37**(4), 1103-1108.
7. Hustert, K. et al *Chemosphere* 1997, **35**(1-2), 33-37.
8. Perkov, W. *Wirksubstanzen der Pflanzenschutz- und Schaedlingsbekämpfungsmittel* 1971/76, Verlag Paul Parey, Berlin, Germany.
9. Hess, C. et al *Proc. Br. Insect. Fungic. Conf.* 1975, **2**, 693.
10. Rankin, G. O. et al *Toxicology* 1989, **56**(3), 263-272.
11. *US Office of Pesticide Programs List of Chemicals Evaluated for Carcinogenic Potential* 1996, US Environmental Protection Agency, Washington, DC 20460, USA.
12. Kelce, W. R. et al *Toxicol. Appl. Pharmacol.* 1994, **126**, 276-285.
13. Gray, L. E. et al *Toxicol. Appl. Pharmacol.* 1994, **129**, 46-52.
14. Dean, G. M. et al *Proc. Br. Crop Prot. Conf. – Pests Diss.* 1988, **2**, 693-698.
15. Chiesara, E. et al *Arch. Toxicol., Suppl.* 1982, (5), 345.
16. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
17. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
18. *1967 Directive on Classification, Packaging and Labelling of Dangerous Substances* 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
19. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
20. *Special Report on Environmental Endocrine Disruption: An Effects Assessment and Analysis* 1997, EPA/630/R-96/012, Risk Assessment Forum, US Environmental Protection Agency, Washington, DC 20460, USA

v24 vincristine



$C_{46}H_{56}N_4O_{10}$

Mol. Wt. 824.97

CAS Registry No. 57-22-7

Synonyms LCR; leurocristine; NCI-C04864; 22-oxovincal leukoblastine; VCR

EINECS No. 200-318-1

RTECS No. OH 6300000

Uses Antineoplastic agent.

Occurrence Alkaloid found in *Vinca rosea*.

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat, mouse 1.25, 4.7 mg kg⁻¹, respectively (1-5).

LD₅₀ intravenous rat, mouse 1.0, 3.0 mg kg⁻¹, respectively (4-7).

LD_{Lo} intravenous woman 40 µg kg⁻¹ (8).

Sub-acute and sub-chronic data

Intravenous rabbit 0.3 mg kg⁻¹ wk⁻¹ for 5 wk. Reduced body weight gain was evident from first injection. Gross signs of motor paralysis and pain were evident from wk 3. At the end of the study, blood analysis revealed normocytic normochromic anaemia, elevated serum creatine kinase and low serum alkaline phosphatase activities. All tested parameters related to the liver and kidneys were normal (9).

Teratogenicity and reproductive effects

Intraperitoneal rat, lowest toxic dose 125 µg kg⁻¹ day⁻¹ on days 6-15 of gestation caused reduced litter size, foetal death and teratogenic effects (10).

Intraperitoneal ♂ mouse, single dose of 0.5-2.0 mg kg⁻¹ reduced the rate of germ cell development and resulted in killing of the non-proliferating spermatid cells (11).

Intravenous golden hamster 0.1 or 0.5 mg kg⁻¹ on day 8 of gestation. 23% resorptions occurred with the low dose and 85% with the high dose. The 6% incidence of foetal abnormalities was not considered to be clearly treatment related (12).

Metabolism and toxicokinetics

Following intraperitoneal administration to rats and mice, peak plasma levels were obtained after 15 min.

Excretion t_{1/2} 60 min in mice, 60-100 min in rats (13,14).

Following intraperitoneal administration to mice, there was a marked accumulation of unchanged drug in the liver, kidneys and spleen; levels were very low in the brain, although metabolite levels were significantly higher than in other organs. After 24 hr radioactivity from tritiated vincristine had fallen in most tissues except the spleen and large intestine, indicating biliary excretion of the drug or metabolites. Over 48 hr, 22% of the dose was excreted in the urine as vincristine and 25% as metabolites. In the faeces, 18% was vincristine and 19% as metabolites (14).

In monkeys, low levels of vincristine and its metabolites rapidly entered the cerebrospinal fluid from the plasma, and persisted for several days (15).

Irritancy

Dermal rabbit (24 hr) 15 mg caused irritation (16).

Genotoxicity

In vitro mouse C3H/10T1/2 clone 8 cells, morphological transformation negative (17).

In vitro human lymphocytes induction of micronuclei and aneuploidy positive (18,19).

In vitro human bone marrow cells sister chromatid exchanges positive (20).

In vivo mouse spermatocytes DNA damage positive (11).

In vivo mouse bone marrow cells induction of micronuclei positive (21).

Other effects

Other adverse effects (human)

Toxic to human erythrocytes *in vitro* (22).

Any other adverse effects

Intraperitoneal mouse single doses of 0.9 or 2.8 mg kg⁻¹ acted as an immunosuppressive agent on the primary cell-mediated immunity when administered after, but not before, allotransplantation antigen (4).

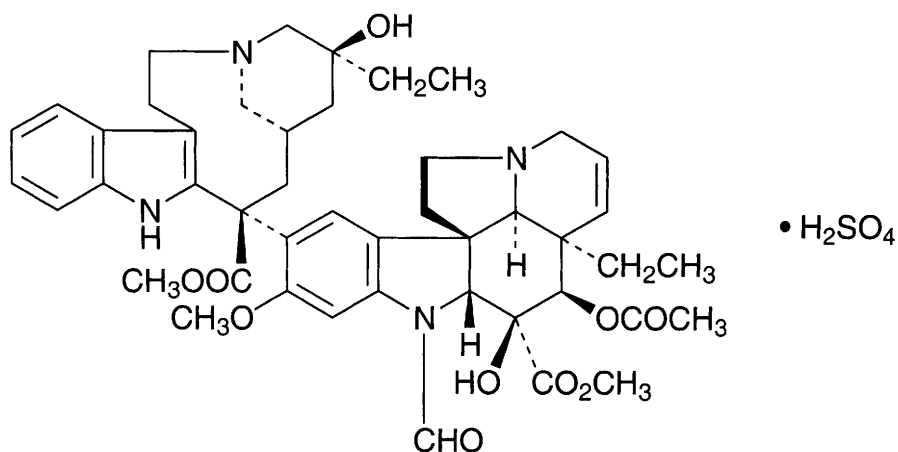
Inhibited protein synthesis in rat liver *in vitro* (23).

Neurotoxicity was demonstrated by histological damage following injection into the dentate gyrus (species unspecified) (24).

References

1. *Med. J. Australia* 1985, **143**, 305.
2. *Adv. Teratol.* 1968, **3**, 181.
3. *Cancer Treat. Rep.* 1981, **65**, 1049.
4. Pyer, M. Y. et al *Saenggyak Hakhoechi* 1986, **17**(3), 248-254 (Korean) (*Chem. Abstr.* **106**, 131406s).
5. Nemeth, L. et al *Neoplasma* 1970, **17**, 345-347.
6. Todd, G. C. et al *Cancer Treat. Rep.* 1979, **63**, 35-41.
7. *J. Med. Chem.* 1985, **28**, 1079.
8. *Cancer Res.* 1979, **39**, 3575.
9. Norido, F. et al *Toxicol. Appl. Pharmacol.* 1988, **93**(3), 433-441.
10. *Ann. Rep. Res. Inst. Environ. Med. Nagoya Univ.* 1967, **15**, 61.
11. Zhang, Y. et al *Mutat. Res.* 1992, **281**, 25-29.
12. Ferm, W. H. *Science* 1963, **141**, 426.
13. Castle, M. C. et al *Cancer Res.* 1976, **36**, 3684-3689.
14. El Dareer, S. M. et al *Cancer Treat. Rep.* 1977, **61**, 1269-1277.
15. Jackson, D. V. et al *Cancer Res.* 1980, **40**, 722-724.
16. *Toxicology* 1979, **14**, 117.
17. Benedict, W. F. et al *Cancer Res.* 1977, **37**, 2202-2208.
18. Eastmond, D. A. et al *Mutat. Res.* 1990, **234**(5), 303-318.
19. Miglione, L. et al *Mutat. Res.* 1989, **227**(3), 167-172.
20. Zhang, S. et al *Cancer Genet. Cytogenet.* 1988, **31**(2), 157-163.
21. Hashimoto, T. et al *J. Toxicol. Sci.* 1987, **12**, 23-32.
22. Sharma, Y. C. et al *Indian. J. Cancer Chemother.* 1989, **11**(2), 63-66.
23. Goethals, F. et al *Toxicol. In Vitro* 1990, **4**(4-5), 435-438.
24. Goldschmidt, R. B. et al *Brain Res.* 1989, **486**(1), 133-140 (*Chem. Abstr.* **110**, 226859p)

v25 vincristine sulfate



C₄₆H₅₈N₄O₁₄S

Mol. Wt. 923.05

CAS Registry No. 2068-78-2

Synonyms des-*N*_a-methyl-*N*_a-formylvinblastine sulfate; LCR-sulfate; leurocristine sulfate (1:1); NSC-67574; Oneovin; 22-oxovinaleukoblastine sulfate; VCR sulfate; Vincrisul

EINECS No. 218-190-0

RTECS No. OH 6340000

Uses Antineoplastic agent, usually in combination with other agents (1).

Occurrence Isolated from several members of the plant genus *Catharanthus* (formerly called *Vinca*) (1).

Physical properties

M. Pt. 273-281°C

Solubility Water: 50%. Organic solvents: chloroform, ethanol, methanol

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat, mouse 1.9, 5.2 mg kg⁻¹, respectively (2,3).

LD₅₀ intravenous rat, mouse 1.0, 2.1 mg kg⁻¹, respectively (2-4).

In rats, the toxic effects included hind-limb paralysis, diuresis, weight loss, dyspnoea, diarrhoea and anorexia (2).

Sub-acute and sub-chronic data

Intravenous dog (6 wk) 0.02, 0.04 or 0.08 mg kg⁻¹ wk⁻¹. With the highest dose, 2/4 animals died with extensive damage to the gut, lymphoid hypoplasia and maturation arrest of spermatocytes. The 2 survivors had no drug-induced lesions at necropsy 44 and 97 days after the start of treatment, respectively. Non-specific lesions of the nervous system occurred with all dose levels (5).

Intravenous monkey (6 wk) 0.08, 0.16, 0.32 or 0.64 mg kg⁻¹ wk⁻¹. 1/2 high-dose monkeys died; both animals had swollen neurons in the ventral horn of the spinal cord and severe damage to the intestinal mucosa. Dose-dependent leucopenia, anaemia and reticulocytosis were reported in animals administered the lower doses (5).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (6).

Intraperitoneal mouse (15 month) 0.075 or 0.15 mg kg⁻¹ 3 × wk⁻¹ for 6 months. Survival was 34-55% that of controls in ♂ mice, and 97-100% that of controls in ♀ mice. Tumour incidences were not significantly different from controls (7).

Intraperitoneal rat (15 month) 0.06 or 0.12 mg kg⁻¹ 3 × wk⁻¹ for 6 months. Survival was 19-100% that of controls in ♂ rats, and 100% that of control in ♀ rats. Tumour incidences were not significantly different from controls (7).

Teratogenicity and reproductive effects

Intravenous ♂ rat, lowest toxic dose 1.25 mg kg⁻¹ day⁻¹ for 10 days, toxic effects at higher doses on testes, prostate and seminal vesicles (8).

Intraperitoneal mouse, lowest toxic dose 0.3 mg kg⁻¹ day⁻¹ for 8 days during gestation – teratogenic effects on central nervous system and craniofacial area (9).

Intraperitoneal mouse, lowest toxic dose 0.25 mg kg⁻¹ day⁻¹ for 9 days, during gestation - foetotoxicity and teratogenic effects to central nervous system, craniofacial area and musculoskeletal system (10).

Genotoxicity

Salmonella typhimurium TA98, TA100 with and without metabolic activation negative (11).

Drosophila melanogaster sex-linked recessive lethal assay negative (12).

In vitro mouse lymphoma L5178Y cells, tk⁺tk⁻ forward mutation assay positive (metabolic activation unspecified) (13).

In vitro Chinese hamster ovary cells, chromosomal aberrations negative (14).

In vitro Syrian hamster fibroblasts and human fibroblasts, induction of aneuploidy positive (15).

In vitro human lymphocytes, micronuclei (prevalently centromere positive) and chromosome nondisjunction positive (16).

In vivo mouse micronucleus assay positive (effects unspecified) (17).

Other effects

Other adverse effects (human)

Intensive combination therapy with regimens including vincristine sulfate has been shown to result in increased risks for acute nonlymphocytic leukaemia. Such combinations usually include procarbazine together with an alkylating agent such as nitrogen mustard, both of which are potential carcinogens. In the presence of concurrent therapy with other putative carcinogens, including ionising radiation and other potent drugs, occasional case reports of exposure to vincristine sulfate do not constitute evidence of carcinogenesis (5).

Other comments

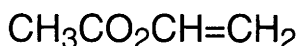
Physical properties, uses, occurrence, analysis, carcinogenicity, mammalian toxicity, metabolism and mutagenicity reviewed (1).

Antineoplastic action is through arrest of cells in metaphase by an effect on microtubules (18).

References

1. IARC Monograph 1981, **26**, 365-384.
2. Adamson, R. H. et al *Arch. Int. Pharmacodyn.* 1965, **157**, 299-311.
3. *Drugs in Japan. Ethical Drugs* 6th ed., 1982, 648, Jokugyo Jiho Co, Tokyo, Japan.
4. *Kiso to Rinsho* 1983, **14**, 1349.
5. Folk, R. M. et al *Cancer Chemother. Repl. Part 3* 1974, **5**, 17-23.
6. IARC Monograph 1987, **Suppl. 7**, 372-373.
7. Weisburger, E. K. *Cancer* 1977, **40**, 1935-1949.
8. *Kiso to Rinsho* 1983, **17**, 1859.
9. *Arch. d'Anatom. d'Histol d'Embryol.* 1965, **48**, 181.
10. Joneja, et al *Teratology* 1969, **2**, 235.
11. Seino, Y. et al *Cancer Res.* 1978, **38**, 2148-2156.
12. Todd, N. et al *Mutat. Res.* 1983, **120**, 121-125.
13. Matheson, D. et al *Drug. Chem. Toxicol.* 1978, **1**, 277-304.
14. Au, W. W. et al *Environ. Mol. Mutagen.* 1980, **2**, 455-464.
15. Tsutsui, T. et al *Mutat. Res.* 1990, **240**, 241-249.
16. Sgura, A. et al *Mutat. Res.* 1997, **392**(1,2), 97-107.
17. Hayashi, M. et al *Mutat. Res.* 1989, **223**(4), 329-344.
18. Greasey, W. A. in Sartorelli, A. C. et al (Eds.) *Antineoplastic and Immunosuppressive Agents 1975 Part II* 670-694, Springer, New York, NY, USA

v26 vinyl acetate



C₄H₆O₂

Mol. Wt. 86.09

CAS Registry No. 108-05-4

Synonyms acetic acid ethenyl ester; acetic acid vinyl ester; 1-acetoxyethylene; ethenyl acetate; vinyl A monomer; ethanoic acid, vinyl ester; VAC; VYAC; Zeset T

EINECS No. 203-545-4

RTECS No. AK 0875000

Uses Manufacture of polymers. Polyvinyl acetate emulsions are used in adhesives and paints, as starch substitute in textile sizings and as binding agent in paper.

Physical properties

M. Pt. -93°C **B. Pt.** 72-73°C **Flash point** -6°C **Specific gravity** 0.9317 at 20°C with respect to water at 4°C

Partition coefficient log P_{ow} 0.73 **Volatility** v.p. 100 mmHg at 21.5°C ; v.den. 3.0

Solubility Water: 20 g l⁻¹ at 20°C. Organic solvents: acetone, benzene, chloroform, diethyl ether, ethanol

Occupational exposure

DE-MAK 10 ppm (36 mg m⁻³)

FR-VME 10 ppm (30 mg m⁻³)

SE-LEVL 5 ppm (18 mg m⁻³)

UK-LTEL 10 ppm (36 mg m⁻³)

US-TWA 10 ppm (35 mg m⁻³)

SE-STEL 10 ppm (35 mg m⁻³)

UK-STEL 20 ppm (72 mg m⁻³)

US-STEL 15 ppm (53 mg m⁻³)

UN No. 1301 (inhibited) HAZCHEM Code 3WE (inhibited) Conveyance classification flammable liquid (inhibited)

Supply classification highly flammable

Risk phrases Highly flammable (R11)

Safety phrases Keep out of reach of children (if sold to general public) – Keep away from sources of ignition – No smoking – Do not breathe vapour – Do not empty into drains – Take precautionary measures against static discharges (S2, S16, S23, S29, S33)

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) golden orfe 28 mg l⁻¹ – static bioassay (1).

LC₅₀ (96 hr) fathead minnow, bluegill sunfish, goldfish, guppy 18-31 mg l⁻¹ (2).

Invertebrate toxicity

IC₅₀ (24 hr) *Daphnia magna* 52 mg l⁻¹ (3).

Toxicity threshold (cell multiplication inhibition test) *Pseudomonas putida* 6 mg l⁻¹, *Scenedesmus quadricauda* 370 mg l⁻¹, *Entosiphon sulcatum* 81 mg l⁻¹ (4).

Bioaccumulation

Estimated bioconcentration factor 2.1-2.4 indicates that environmental accumulation is unlikely (5).

Environmental fate

Nitrification inhibition

Not inhibitory to nitrifying bacteria at 100 mg l⁻¹ (6).

Degradation studies

BOD₅ 42% of ThOD in marine water, 51% of ThOD in sewage inocula (7).

Abiotic removal

Hydrolysis t_{1/2} 7.3 days at pH 7. Rate of hydrolysis increases with pH (8).

Undergoes polymerisation in light (9).

Reacts with photochemically produced hydroxyl radicals in the atmosphere, estimated t_{1/2} 14.6 hr (10).

Volatilisation t_{1/2} 4.4 hr for model river water, 2.1 days for model pond water (5,11).

Adsorption by activated carbon 129 mg g⁻¹ carbon; influent concentration 1000 mg l⁻¹, effluent 360 mg l⁻¹ (12).

Adsorption and retention

Estimated K_{oc} 19-59 indicate that adsorption to soil and sediment would not be significant (5).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 1600, 2900 mg kg⁻¹, respectively (13,14).

LC₅₀ (4 hr) inhalation mouse, rabbit 1550, 2500 ppm, respectively (15,16).

LC₅₀ (2 hr) inhalation rat 4000 ppm (17).

LD₅₀ dermal rabbit 2335 mg kg⁻¹ (15).

Sub-acute and sub-chronic data

Inhalation rat, mouse (3 month) 1000 ppm for 6 hr day⁻¹ 6 day wk⁻¹ caused a reduction in body-weight gain. No specific damage to parenchymal organs was noted (18).

Inhalation rat (6 month) 3-140 ppm caused a slight but dose-dependent decrease in hepatic microsomal cytochrome P₄₅₀ level (19).

Inhalation rat (4 wk) 0, 5, 20, 600, or 1000 ppm for 1, 5, or 20 exposures. Rats were killed 18 hr after the last exposure for evaluation of nasal epithelial cell proliferation. The results demonstrated the capability for distinctly different responses between respiratory and olfactory epithelium and suggested a role for cellular and biochemical adaptation in the toxic response to vinyl acetate exposure. The no-observed-adverse-effect level for all effects was 20 ppm (20).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (21).

Oral rat (130 wk) 0, 1000 or 2500 mg l⁻¹ in drinking water for 100 wk. At that time, survival in ♂ and ♀ was 7/20 and 5/20 in controls, 8/20 and 11/20 in low-dose group, and 6/20 and 11/20 in high-dose group, respectively. The incidences of liver neoplastic nodules were: 0 in controls, 4 low-dose and 2 high-dose ♂; 0 in controls, 0 low-dose and 6 high-dose ♀; of uterine adenocarcinoma: 0 in controls, 1 low-dose and 5 high-dose ♀; of uterine polyps: 0 in controls, 3 low-dose and 6 high-dose ♀; of thyroid C-cell adenoma 0 in controls, 3 low-dose and 5 high-dose ♀ (22).

Inhalation rat (135 wk) 8800 mg m⁻³ 4 hr day⁻¹ 5 day wk⁻¹ for 52 wk (maximum tolerated concentration). No tumours were reported. Early mortality was high, only 49/96 animals survived for ≥26 wk (23).

Teratogenicity and reproductive effects

Oral ♂ rat, lowest toxic dose 500 mg kg⁻¹ day⁻¹ in multigeneration study, reduced fertility index (24).

Oral ♂ rat, 125 and 500 mg kg⁻¹ day⁻¹ for 5 days caused a reduction in testicular weight (25).

Inhalation ♀ rat (days 6-15 of gestation, 6 hr day⁻¹) 0-1000 ppm. Maternal and foetal toxicity were observed at 1000 ppm. The no-observed-effect level was 200 ppm (26).

Metabolism and toxicokinetics

Rats exposed to vinyl acetate exhaled acetaldehyde, as a result of hydrolysis by esterases (27).

When mice were exposed to ¹⁴C-vinyl acetate, the radioactivity excretion pattern was similar to that observed with ¹⁴C-acetaldehyde. The majority of radioactivity was exhaled as ¹⁴CO₂ (28).

In vitro, vinyl acetate is metabolised mainly by hydrolysis to acetaldehyde and acetic acid. Esterases present in whole blood in plasma of rats and mice and those present in the liver and lung catalyse the reaction (27,28).

Rat liver supernatant catalyses conjugation of vinyl acetate with glutathione. Accordingly, doses of ~500 mg kg⁻¹ have led to a slight reduction in hepatic glutathione levels in rats and some other species (29,30).

Irritancy

Dermal rabbit (24 hr-open) 10 mg caused irritation (31).

500 mg instilled into rabbit eye for 24 hr caused mild irritation (32).

Inhalation rat, mouse (4 wk) 500 ppm in rats and 150 ppm in mice for 6 hr day⁻¹ caused signs of respiratory tract irritation (28).

Inhalation rat (3 wk) 2000 ppm for 6 hr day⁻¹ caused irritation of the eyes and nose and respiratory difficulty (33).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537, TA1538 with and without metabolic activation negative (34).

Induced the transformation of Syrian hamster cells by adenovirus SA7 (35).

In vitro Chinese hamster ovary cells sister chromatid exchanges with metabolic activation positive (36,37).

In vitro human isolated lymphocytes and whole blood cultures sister chromatid exchanges and chromosomal aberrations positive (metabolic activation unspecified) (37).

In vitro mouse sperm morphology abnormalities positive, induction of meiotic micronuclei negative (25).

Other effects

Other adverse effects (human)

Exposure of four volunteers indicated that irritation of the mucous membranes can occur at 20 ppm, and eye irritation at 72 ppm (38).

Impairment of ventilatory function and symptoms of chronic bronchitis have been reported among workers exposed to up to 40 ppm, although workers were exposed to other chemicals such as various aldehydes and vinyl copolymers (39,40).

Among 558 exposed workers, liver function changes were reported in the majority. Neurological disorders were reported to occur 6 times more frequently among workers in the vinyl acetate production department than in an unspecified control group. No increase was noted in workers in other departments. Overall, 25% of production workers had skin disorders (41).

The increased lung cancer risk observed in a synthetic chemical plant, in which vinyl acetate was 1 of 19 chemicals considered, could not be associated specifically with exposure to vinyl acetate (42).

Other comments

Detected in natural water and air samples (43).

Environmental fate reviewed (43).

Physical properties, uses, occurrence, analysis, carcinogenicity, mammalian toxicity, metabolism and mutagenicity reviewed (44-48).

Unlike other vinylic monomers, the biological effects of vinyl acetate may be due to its hydrolysis to acetaldehyde, rather than to epoxidation of the vinyl moiety (48).

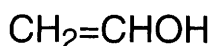
Autoignition temperature 427°C.

References

1. Kurllet, M. J. et al *Environ. Sci. Technol.* 1987, **21**(2), 149-155.
2. Pickering, G. H. et al *J. Water Pollut. Control Fed.* 1966, **38**(9), 1419.
3. Devillers, J. et al *Chemosphere* 1987, **16**(6), 1149-1163.
4. Bringmann, G. et al *Water Res.* 1980, **14**, 231-241.
5. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
6. Arenshtein, A. M. *Biokhim. Och. Stockn.* 1962, 128-177 (*Chem. Abstr.* **61**, 15067).
7. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
8. Takemoto, S. et al *Suishitsu Odaku Kenkyu* 1981, **4**, 80-90.
9. Mabey, W. et al *J. Phys. Chem. Ref. Data* 1978, **7**, 383-415.
10. Atkinson, R. *Int. J. Chem. Kinet.* 1987, **19**, 799-828.
11. *EXAMS II Computer Simulation* 1987, US EPA, Athens, GA, USA.
12. Guisti, D. M. et al *J. Water Pollut. Control Fed.* 1974, **16**(5), 947-965.
13. *Union Carbide Data Sheet* 25 Apr 1958, Union Carbide Corp., New York, NY, USA.
14. *Gig. Sanit.* 1966, **31**(8), 19.
15. *DuPont Technical Sheet* 1975, ES-3574, DuPont de Nemours, Wilmington, DE, USA.
16. *Documentation of Threshold Limit Values and Biological Exposure Indices* 5th ed., 1986, 621, American Conference of Governmental Industrial Hygienist Inc., Cincinnati, OH, USA.
17. Union Carbide Corp. *Special Report* 36-72 1973, Danburg, CT, USA.
18. Owen, P. E. et al *Human Toxicol.* 1983, **2**, 416.
19. Holub, J. *Przegl. Lek.* 1983, **40**, 515-516.
20. Bogdanffy, M. S. *Inhalation Toxicol.* 1997, **9**(4), 331-350.
21. *IARC Monograph* 1987, **Suppl. 7**, 73.
22. Lijinsky, W. et al *Toxicol. Appl. Pharmacol.* 1983, **68**, 43-53.
23. Maltoni, C. et al *Ann. N.Y. Acad. Sci.* 1975, **246**, 195-218.
24. *Report* US EPA, 8EH9-0185-0543, Office of Pesticides and Toxic Substances, Washington, DC, USA.
25. Lahdetie, J. *Mutat. Res.* 1988, **202**(1), 171-178.
26. Hurtt, M. E. et al *Fundam. Appl. Toxicol.* 1995, **24**(2), 198-205.
27. Simon, P. et al *Arch. Toxicol.* 1985, **57** 19-23.
28. Hazleton Laboratories Europe *Vinyl Acetate: Compilation of Data* in Herschler, D. (Ed.) *Gesundheitsschadliche Arbeitsstoffe. Toxikologisch/Arbeitsmedizinische Begründungen von MAK – Werten* 1979, Verlag Chemie, Weinheim, Germany.
29. Boyland, E. et al *Biochem. Pharmacol.* 1970, **19**, 1526-1528.
30. Holub, J. et al *Ind. Arch. Occup. Environ. Health* 1982, **51**, 185-189.
31. Smyth, H. F. et al *J. Ind. Hyg. Toxicol.* 1948, **30**, 63.
32. Marhold, J. V. *Prehled Prumyslove Toxikologie: Organické Latky* 1986, Prague, Czechoslovakia.
33. Gage, J. C. *Br. J. Ind. Med.* 1970, **27**, 1-18.
34. Klopman, G. et al *Mutat. Res.* 1990, **228**(1), 1-50.
35. Casto, B. C. et al *Proc. Am. Assoc. Cancer Res.* 1977, **18**, 155.
36. Jartunen, K. et al *Mutat. Res.* 1986, **159**, 109-116.
37. Norppa, H. et al *Cancer Res.* 1985, **45**, 4816-4821.
38. *Criteria for a Recommended Standard for Occupational Exposure to Vinyl Acetate* 1978, National Institute for Occupational Safety and Health DHEW (NIOSH) Publ. No. 78-205, Cincinnati, OH, USA.

39. Ahoronian, Z. P. et al *Zh. Eksp. Klin. Med.* 1982, **22**, 151-155.
40. Jedrychowski, W. et al *Przegl. Lek.* 1979, **36**, 679-682.
41. Nargizyan, G. A. et al *Zh. Eksp. Klin. Med.* 1978, **18**, 101-104.
42. Wascweiler, R. J. et al *Environ. Health Perspect.* 1981, **41**, 159-165.
43. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1989, **1**, 545-550, Lewis Publ., Chelsea, MI, USA.
44. Sentodonata, J. *Report* 1985, SRC-TR-85-190, Order No. PB 86-155157/GAR, NTIS, Washington, DC, USA.
45. *Chemical Safety Data Sheets* 1992, **5**, 264-267, The Royal Society of Chemistry, London, UK.
46. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
47. Clary, J. J. *Ann. N. Y. Acad. Sci.* 1988, **534**, 255-260.
48. *IARC Monograph* 1986, **39**, 113-131

v27 vinyl alcohol



$\text{C}_2\text{H}_4\text{O}$

Mol. Wt. 44.05

CAS Registry No. 557-75-5

Synonyms ethenol; hydroxyethene; hydroxyethylene

EINECS No. 209-183-3

RTECS No. YZ 0495000

Uses Manufacture of polymers.

Occurrence Enol tautomer of acetaldehyde, not known in the free state.

Mammalian & avian toxicity

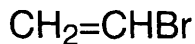
Acute data

LD₅₀ oral rat 64 mg kg⁻¹ (1).

References

1. *J. Pharm. Sci.* 1974, **63**, 1068

v28 vinyl bromide



$\text{C}_2\text{H}_3\text{Br}$

Mol. Wt. 106.95

CAS Registry No. 593-60-2

Synonyms bromoethene; bromoethylene; NCI-C50373

EINECS No. 209-800-6

RTECS No. KU 8400000

Uses Manufacture of polymers, flame retardants, pharmaceuticals and fumigants.

Physical properties

M. Pt. -139°C B. Pt. 16°C at 750 mmHg Flash point <-18°C (closed cup) Specific gravity 1.51 at 20°C with respect to water at 4°C Volatility v.p. 895 mmHg at 20°C ; v.den. 3.7

Solubility Organic solvents: acetone, benzene, chloroform, diethyl ether, ethanol

Occupational exposure

US-TWA 0.5 ppm

UN No. 1085 (inhibited) HAZCHEM Code 2WE (inhibited) Conveyance classification flammable gas (inhibited)

Supply classification extremely flammable

Supply classification toxic

Risk phrases Extremely flammable – May cause cancer (R12, R45)

Safety phrases Avoid exposure – obtain special instruction before use – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S53, S45)

Environmental fate

Abiotic removal

Undergoes rapid polymerisation in sunlight (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 500 mg kg⁻¹ (2).

LC_{Lo} (7 hr) inhalation rat 50,000 ppm (3).

Sub-acute and sub-chronic data

Inhalation rat (4 wk) 10,000 ppm 7 hr day⁻¹ 5 day wk⁻¹ caused no significant adverse effects (4).

Inhalation newborn rat 2000 ppm 8 hr day⁻¹ 5 days wk⁻¹ for 18-15 wk induced the development of ATPase-deficient foci in the liver, but to an extent ~10 times lower than that for vinyl chloride (5,6).

Inhalation rat 20,000 ppm 4 hr day⁻¹ for 10 days caused a decrease in hepatic cytochrome P₄₅₀ content (7).

Carcinogenicity and chronic effects

Limited evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2A (8).

Dermal mouse 15 mg animal⁻¹ 3 × wk⁻¹ for 60 wk induced no observable tumour. In a two-stage initiating study, mice received a single application of vinyl bromide followed by 2.5 µg 12-*O*-tetradecanoylphorbol 13-acetate (TPA) 3 × wk⁻¹ for 60 wk, a single application of 7,12-dimethylbenz[*a*]anthracene (DMBA) followed by treatment with TPA, treatment with TPA, only, or no treatment at all. 1/30 mice treated with vinyl bromide/TPA developed a skin papilloma at 412 days, 1/30 TPA-treated mice developed a skin carcinoma after 44 days, no skin tumour developed in 160 untreated controls within 420 days, and the DMBA positive control group showed the expected high incidence of skin tumours (9).

Subcutaneous mouse (60 wk) 25 mg animal⁻¹ 2 × wk⁻¹. No local tumour was observed in treated animals or in controls (9).

Inhalation rat 0, 10, 50, 250 or 1250 ppm 6 hr day⁻¹ 5 day wk⁻¹ for 104 wk caused a dose-related incidence of angiosarcomas and Zymbal gland carcinomas. An increased incidence of liver neoplastic nodules and hepatocellular carcinoma was also noted (10).

Metabolism and toxicokinetics

Readily absorbed by the lungs in rats. Metabolism was saturable at exposure concentration >55 ppm and was associated with the release of bromide into the plasma (11,12).

In vitro studies indicate that the primary metabolite formed by mixed-function oxidases is 2-bromoethylene oxide. Its rearrangement product, 2-bromoethanol is believed to be the major alkylating agent bound to protein (13). When incubated with liver microsomes from phenobarbital-treated rats, vinyl bromide alkylated the prosthetic group (haem) of cytochrome P₄₅₀. The alkylated moiety has been identified as the dimethyl ester of *N*-(2-oxoethyl)protoporphyrin IX (14).

Irritancy

Irritating to skin and eyes (species unspecified) (15).

Genotoxicity

Salmonella typhimurium TA98, TA100 with metabolic activation positive (16,17).

Other effects

Other adverse effects (human)

Short-term inhalation of high concentrations (unspecified) caused loss of consciousness. Skin and eye contact with liquid vinyl bromide produced irritation and caused a "frost-bite" type of burn (10,18).

Other comments

Physical properties, uses, occurrence, analysis, carcinogenicity, mammalian toxicity, metabolism and mutagenicity reviewed (19-21).

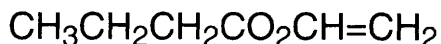
Formulations include ~200 ppm hydroquinone monomethyl ether as inhibitor.

Autoignition temperature 530°C.

References

1. Buckingham, J. (Ed.) *Dictionary of Organic Compounds* 5th ed., 1982, 1, 799, Chapman and Hall, London, UK.
2. Dow Chemical Co. *Report* 1966, 12, Midland, MI, USA.
3. *Documentation of Threshold Limit Values and Biological Exposure Indices* 5th ed., 1986, American Conference of Governmental Industrial Hygienists, Cincinnati, OH, USA.
4. Leong, B. K. J. et al *Am. Ind. Hyg. Assoc. J.* 1970, **31**, 1-11.
5. Bolt, H. M. et al *Arch. Toxicol.* 1979, **43**, 83-84.
6. Bolt, H. M. et al *Biochem. Pharmacol.* 1982, **31**, 1-4.
7. Drew, R. T. et al *Toxicol. Appl. Pharmacol.* 1976, **37**, 176-177.
8. *IARC Monograph* 1987, **Suppl. 7**, 73.
9. van Duuren, B. L. *Environ. Health Perspect.* 1977, **21**, 17-23.
10. Benya, T. J. et al *Toxicol. Appl. Pharmacol.* 1982, **64**, 367-377.
11. Filser, J. G. et al *Arch. Toxicol.* 1979, **42**, 123-136.
12. Gargas, M. L. et al *Toxicol. Appl. Pharmacol.* 1982, **66**, 55-68.
13. Geungerich, F. P. et al *Cancer Res.* 1982, **41**, 4391-4398.
14. Ortiz de Montelleno, P. P. et al *Biochemistry* 1982, **21**, 1331-1339.
15. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, 2, 3600, Sigma-Aldrich, Milwaukee, WI, USA.
16. Bartsch, H. et al *Proc. Am. Assoc. Cancer Res.* 1976, 17, 17.
17. Lijinsky, W. et al *Teratog., Carcinog., Mutagen.* 1980, **1**, 259-267.
18. Fawcett, H. H. *Investigation of Agents which are Newly Suspected as Occupational Health Hazards, Vinyl Halides* 1976, 9-12, Tracor Jiteo, Rockville, MD, USA.
19. *IARC Monograph* 1986, **39**, 133-145.
20. *Chemical Safety Data Sheets* 1982, 5, 268-270, The Royal Society of Chemistry, London, UK.
21. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

v29 vinyl butyrate



C₆H₁₀O₂

Mol. Wt. 114.14

CAS Registry No. 123-20-6

Synonyms ethenyl butanoate

EINECS No. 204-609-4

RTECS No. ET 7000000

Uses Organic synthesis.

Physical properties

B. Pt. 116°C **Flash point** 20°C (open cup) **Specific gravity** 0.9 **Volatility** v.den. 4.0

Occupational exposure

UN No. 2838 (inhibited) **HAZCHEM Code** 3WE (inhibited) **Conveyance classification** flammable liquid (inhibited)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 8500 mg kg⁻¹ (1).

LC_{Lo} (4 hr) inhalation rat 4000 ppm (2).

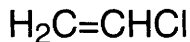
Irritancy

Dermal rabbit 500 mg caused mild irritation and 500 mg instilled into rabbit eye caused irritation (exposure unspecified) (1,2).

References

1. *Union Carbide Data Sheet* 24 March 1970, Union Carbide Corp., New York, NY, USA.
2. *AMA Arch. Ind. Hyg. Occup. Med.* 1951, 4, 119

v30 vinyl chloride



C₂H₃Cl

Mol. Wt. 62.50

CAS Registry No. 75-01-4

Synonyms chloroethylene; chloroethene; ethylene monochloride; monochloroethylene; vinyl chloride monomer

EINECS No. 200-831-0

RTECS No. KU 9625000

Uses Intermediate in the production of chlorinated compounds. Refrigerant gas. Plastics industry.

Physical properties

M. Pt. -153.7°C **B. Pt.** -13.9°C **Flash point** -61°C (1) **Specific gravity** 0.9121 at 15°C with respect to water at 4°C **Partition coefficient** log P_{ow} 1.36 **Volatility** v.p. 2660 mmHg at 25°C ; v.den. 2.15

Solubility Water: 1.1 mg l⁻¹ at 25°C. Organic solvents: benzene, chlorinated solvents, diethyl ether, ethanol

Occupational exposure

FR-VME 1 ppm (plants after 1980); 3 ppm (plants before 1980)

JP-OEL 2.5 ppm (6.5 mg m⁻³)

SE-LEVL 1 ppm (2.5 mg m⁻³)

SE-STEL 5 ppm (13 mg m⁻³)

UK-LTEL MEL 7 ppm; 3 ppm (annual exposure limit)

US-TWA 1 ppm

UN No. 1086 **HAZCHEM Code** 2WE **Conveyance classification** flammable gas

Supply classification extremely flammable, toxic

Risk phrases May cause cancer – Extremely flammable (R45, R12)

Safety phrases Restricted to professional users – Avoid exposure – obtain special instruction before use – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S53, S45)

Ecotoxicity

Bioaccumulation

Not expected to hydrolyse, bioaccumulate in aquatic organisms, or adsorb onto sediments if released into water (2).

Environmental fate

Degradation studies

Resistant to microbial degradation under aerobic conditions (2).

Mycobacterium aureum L1 is capable of growth on vinyl chloride as a sole carbon source (3).

In a mixed methanotrophic culture grown under copper deficiency with 10 mM formate present, 0.85 μmol of vinyl chloride was transformed mg^{-1} cells. Aquifer microcosms transformed up to 4.8 mg l^{-1} with no apparent toxic effects. Around 25 \times more vinyl chloride was transformed in the soil organisms unit $^{-1}$ methane consumed than in aqueous batch tests (4).

Resting cell suspensions of a soil *Pseudomonas* sp. readily metabolise vinyl chloride. The rate of Cl^{-} liberation is a function of growth conditions. Cells grown on 3-chloropropanol carry out the dehalogenation of vinyl chloride with a $t_{1/2}$ of 1.3 hr at a cell density of 0.1 g ml^{-1} (5).

Abiotic removal

If released into soil, subject to rapid volatilisation; reported $t_{1/2}$ 5 hr and 12 hr for evaporation from soil at 1 and 10 cm depth, respectively (6).

Volatilisation from ponds, lakes and rivers, $t_{1/2}$ 43.3, 34.7 and 8.7 hr, respectively. Hydrolytic $t_{1/2} \leq 10$ yr (6).

Adsorption and retention

Does not adsorb significantly to suspended solids and sediments in water (2).

The soil adsorption coefficient has been estimated to range between 17 and 131. Therefore, expected to be highly mobile in soil and leach into ground water (2).

Mammalian & avian toxicity

Acute data

LD_{50} oral rat 500 mg kg^{-1} (7).

Carcinogenicity and chronic effects

Sufficient evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 1 (8).

σ° and f rats (1 yr) exposed to 30,000 ppm developed liver angiosarcomas (9).

Oral σ° and f rats (149 wk) 0-1.3 $\text{mg vinyl chloride monomer (VCM) kg}^{-1}$ body weight day^{-1} . There was no evidence that feeding of VCM affected the incidence of tumours in organs other than the liver. Feeding of VCM at a level of 1.3 mg kg^{-1} body wt. can induce neoplastic and non-neoplastic changes in the livers of σ° and f rats.

Feeding of 0.014 or 0.13 mg kg^{-1} may result in an increased incidence of (basophilic) foci of cellular alteration in the liver of f rats. The no-observed-adverse-effect level for the induction of tumours in rats was concluded to be 0.13 mg VCM kg^{-1} body weight day^{-1} (10).

Teratogenicity and reproductive effects

TD_{Lo} (26 wk) inhalation rat 100 ppm 6 hr day^{-1} caused σ° , paternal effects (11).

TC_{Lo} (1-9 days pregnant) inhalation rat 1500 ppm for 24 hr affected fertility (12).

2736 workers in 13 polyvinyl chloride factories in China were investigated for reproductive function. The results for σ° workers were not significant, however f workers showed an increase in pregnancy complications (13).

Metabolism and toxicokinetics

Predominant human urinary metabolite is thiodiglycolic acid (14).

Inhalation rat (concentration and duration unspecified) polar metabolites, 2-chloroacetic acid, *N*-acetyl-*S*-(2-hydroxyethyl) cysteine, *N*-acetyl-*S*-(2-chloroethyl) cysteine, 2-chloroacetic acid, thiodiglycolic acid and glutamic acid excreted in urine (15).

Genotoxicity

Salmonella typhimurium TA100 with and without metabolic activation positive (16).

Mutagenic effects in man were studied in lymphocyte culture with 3 assays; chromosomal aberration, micronuclei, and sister chromatid exchange. Compared with controls, values are increased in workers occupationally exposed to vinyl chloride (17).

Other effects

Other adverse effects (human)

A large number of epidemiological studies and case reports have substantiated the causal association between vinyl chloride and angiosarcoma of the liver. Several studies also confirm that exposure to vinyl chloride causes other forms of cancer, i.e. hepatocellular carcinoma, brain tumours, lung tumours, and malignancies of the lymphatic and haematopoietic system (8).

A nine-year follow up study of 28 men occupationally exposed to vinyl chloride monomer detected a significant increase in lymphocyte chromosomal damage and elevated sister chromatid exchange frequencies during the third and fourth years. During the last two years, these parameters were approaching control values as a result of decreasing vinyl chloride monomer concentrations in the working environment (18).

Inhalation human estimated average retention 42% (19).

The course of disease induced by vinyl chloride (VC) in 21 process workers from initial exposure to diagnosis, ultimately to death, and problems that occurred in the elucidation of the true nature of the lesions and the occupational origin have been described. Death was due to malignant hepatoma, predominantly angiosarcoma of the liver in 90% of cases, although hepatocellular and cholangiocellular carcinoma were also observed. Latency periods of 12 to 34 yr with a mean latency of 22 yr, with shorter latency periods associated with first exposure at a young age, namely <27 yr (20).

A study was performed to determine the prevalence and time of appearance of serum anti-p53 antibodies during the pathogenesis of angiosarcoma of the liver (ASL) associated with occupational exposure to vinyl chloride.

Enzyme-linked immunoassay (EIA) was used to detect anti-p53 antibodies in individuals occupationally exposed to vinyl chloride; 15 of these individuals had ASL. It was concluded that serum anti-p53 antibodies can predate clinical diagnosis of certain tumours, such as ASL, and may be useful in identifying individuals as high cancer-risk, such as workers with occupational exposure to vinyl chloride (21).

Any other adverse effects

Crosses the placenta (12).

Animal data suggest that human exposure to xenobiotics and drugs that induce mixed function oxidases may result in increased sensitivity to vinyl chloride (22).

Foetotoxic effects observed in animals, particularly when ethanol was administered simultaneously in the drinking water (23).

Legislation

Covered in the UK by the Control of Carcinogenic Substances, Control of Substances Hazardous to Health Regulations 1988 (24).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds not covered by parameter No. 55: guide level 1 µg l⁻¹ (25).

Included in Schedule 4 (Release into Air: Prescribed Substances) of Statutory Instrument No. 472, 1991 (26).

Other comments

Toxicity and occupational hazards reviewed (27-34).

Mutagenicity, carcinogenicity and reproductive hazards reviewed (35-37).

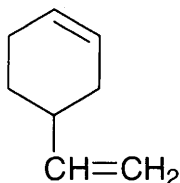
Microbial degradation reviewed (38).

Genetic toxicology reviewed (39).

References

1. *The Sigma-Aldrich Library of Regulatory and Safety Data* 1993, Sigma-Aldrich Corporation, PO Box 355, Milwaukee, USA.
2. Lyman, W. J. et al *Handbook of Chemical Property Estimation Methods* 1982, McGraw-Hill, New York, NY, USA.
3. Hartmans, S. et al *Appl. Environ. Microbiol.* 1992, **58**(4), 1220-1226.
4. Dolan, M. E. et al *Environ. Sci. Technol.* 1995, **29**(11), 2741-2747.
5. Castro, C. E. et al *Environ. Toxicol. Chem.* 1992, **11**(6), 757-764.
6. Jury, W. A. et al *J. Environ. Qual.* 1984, **13**, 573-579.
7. Maltoni, C. et al *Environ. Health Persp.* 1981, **41**, 3.
8. *IARC Monograph* 1987, **Suppl.** 7, 373.
9. Mastromatteo, E. et al *Am. Ind. Hyg. Assoc. J.* 1960, **21** 394.
10. Til, H. P. et al *Food Chem. Toxicol.* 1991, **29**(10), 713-718.
11. Bi, W. et al *Ecotoxicol. Environ. Saf.* 1985, **10**, 281.
12. Ungvary, G. et al *Toxicology* 1978, **11**, 45.
13. Huang, M. *Zhonghua Laodong Weisheng Zhiyebing Zazhi* 1994, **12**(1) (Ch.) (*Chem. Abstr.* 121 090428).
14. Heger, M. et al *Int. Arch. Occup. Environ. Health* 1982, **50**, 187.
15. Hefner, R. E. et al *Ann. N.Y. Acad. Sci* 1975, **246**, 135.
16. Victorin, K. et al *Environ. Mol. Mutagen.* 1988, **11**, 65-77.
17. Fucic, A. et al *Mutat. Res.* 1990, **242**, 265.
18. Fucic, A. et al *Mutat. Res.* 1996, **361**(1), 49-53.
19. Krajewski, J. et al *Br. J. Ind. Med.* 1980, **37**, 373.
20. Lebach, W. K. *Am. J. Ind. Med.* 1996, **29**(5), 446-458.
21. Trivers, G. E. et al *J. Natl. Cancer Inst.* 1995, **87**(18), 1400-1407.
22. Conolly, R. B. et al *Toxicol. Appl. Pharmacol.* 1978, **45**, 338.
23. Clayton, G. D. et al *Patty's Industrial Hygiene and Toxicology* 3rd ed., 1981, **2B**, John Wiley & Sons, New York, NY, USA.
24. *Control of Substances Hazardous to Health and Control of Carcinogenic Substances; Control of Substances Hazardous to Health Regulations 1988 Approved Codes of Practice – 3rd ed.* 1991, HMSO, London, UK.
25. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
26. *S. I.* 1991 No. 472 *Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
27. *Dangerous Prop. Ind. Mater. Rep.* 1989, **9**, 7.
28. Purchase, I. F. H. et al *Food Chem. Toxicol.* 1987, **25**, 187.
29. *Cah. Notes Doc.* 1983, **111**, 297.
30. Nicholson, W. J. et al *Prog. Clin. Biol. Res.* 1984, **4**, 13.
31. Harrison, E. A. *Toxicity of Vinyl Chloride* 1979, Natl. Tech. Inf. Ser., Springfield, VA, USA.
32. Selikoff, I. J. et al *Am. N. Y. Acad. Sci., Vol. 246. Toxicity of Vinyl Chloride-Poly(Vinyl Chloride)*, 1975.
33. Nicholson, W. J. et al *Prog. Clin. Biol. Res.* 1984, **141**, 15B5.
34. Easter, M. D. et al *J. Appl. Toxicol.* 1994, **14**(4), 301-307.
35. Uzych, L. *Hum. Toxicol.* 1988, **7**, 517.
36. Laib, R. J. *IARC Sci. Publ.* 1986, **70**, 101.
37. Kalmaz, E. E. et al *Regul. Toxicol. Pharmacol.* 1984, **4**, 13.
38. Hartmans, S. *Prog. Ind. Microbiol.* 1995, **32**, 239-248.
39. Giri, A. K. *Mutat. Res.* 1995, **339**(1), 1-14

v31 4-vinyl-1-cyclohexene



C₈H₁₂

Mol. Wt. 108.18

CAS Registry No. 100-40-3

Synonyms butadiene dimer; cyclohexenylethylene; 4-ethenyl-1-cyclohexene; NCI-C54999; 1,2,3,4-tetrahydrostyrene; 1-vinylcyclohex-3-ene

EINECS No. 202-848-9

RTECS No. GW 6650000

Uses Manufacture of flame retardants and insecticides. Antioxidant. Organic synthesis.

Physical properties

M. Pt. -101°C **B. Pt.** 126-127°C **Flash point** 20°C (open cup) **Specific gravity** 0.832 at 20°C with respect to water at 4°C **Volatility** v.p. 25.8 mmHg at 38°C ; v.den. 3.76

Solubility Organic solvents: benzene, diethyl ether, light petroleum

Occupational exposure

US-TWA 0.1 ppm (0.44 mg m⁻³)

Environmental fate

Degradation studies

Prolonged exposure to temperatures >26.6°C leads to discoloration and gum formation (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 2600 mg kg⁻¹ (1).

LC₅₀ inhalation rat, mouse 27,000, 47,000 mg m⁻³, respectively (exposure unspecified) (2).

LD₅₀ dermal rabbit 17,000 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

Inhalation rat, mouse 1000 mg m⁻³ 6 hr day⁻¹ for 4 months inhibited body-weight gain and caused leucocytosis, leucopenia, and impaired haemodynamics (2).

Gavage rat, mouse (13 wk) 0-1200 mg kg⁻¹ 5 day wk⁻¹. Hyaline droplet degeneration of the proximal convoluted tubules of the kidneys was observed in ♂ rats, and a reduction in the number of primary follicles and mature Graafian follicles was seen in the ovaries of ♀ mice given the 1200 mg kg⁻¹ dose (3).

Intraperitoneal mouse two doses of 500 mg kg⁻¹ at 24 hr intervals induced liver microsomal NADPH cytochrome c reductase and aminopyrine N-demethylase activities. Liver glutathione depletion was also observed, probably as a result of conjugation of 4-vinylcyclohexene and/or its metabolites (4).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (5).

Gavage rat, mouse 0, 200 or 400 mg kg⁻¹ 5 day wk⁻¹ for 103 wk. Survival rates were: ♂ mice controls 74%, low dose 78%, high dose 14%; ♀ mice 80% controls, 78% low dose, 34% high dose; ♂ rats 64% controls, 26% low dose, 10% high dose; ♀ rats 80% for controls, 56% low dose 26% high dose. In mice there was dose-related increase in ovarian tumours. Increased incidences of benign mixed-cell tumours and adrenal cortical adenomas were also

seen in ♀ mice, and lung tumours and lymphomas in ♂ mice. In rats skin papillomas or carcinomas were observed in ♂, and an increased incidence of clitoral gland adenomas or squamous cell carcinomas was seen in low dose ♀ rats. Non-neoplastic lesions, inflammation and epithelial hyperplasia of the forestomach, lung congestion and atrophy of the red pulp of the spleen in treated mice, and hyperplasia of the forestomach in rats were seen (3).

Dermal ♂ mouse, 45 mg animals $3 \times \text{wk}^{-1}$ for life. Median survival time was 375 days. Skin tumours occurred in 6/20 animals compared with 11/150 controls. Because the 4-vinylcyclohexene used in this study may have been contaminated by autooxidation products, further study was carried out using oxygen free material, administering one fifth of the previously applied dose for life. The median survival time was 565 days. No carcinogenic effect was observed (6).

Gavage ♀ mouse (2 yr) 200 or 400 mg $\text{kg}^{-1} \text{ day}^{-1}$. Survival and mean body weight were reduced in the high-dose groups. A marked increase in the incidences of uncommon ovarian neoplasms, including mixed benign-tumours, granulosa-cell tumours and/or carcinomas was reported in both treatment groups. Increased incidences of a number of non-neoplastic lesions, including mild acute inflammatory lesions and epithelial hyperplasia of the forestomach, congestion of the lungs and adrenal glands at the high dose, and cytological alteration of the adrenal cortex at both doses were also reported. An increased incidence of adrenal gland capsular adenomas in the high-dose group may also have been treatment related (7).

Teratogenicity and reproductive effects

Intraperitoneal ♀ mouse 0, 100, 400 or 800 mg $\text{kg}^{-1} \text{ day}^{-1}$ for 30 days caused ovarian follicle toxicity (8).

Metabolism and toxicokinetics

Rat and mouse liver microsomal mixed-function oxidases metabolise 4-vinyl-1-cyclohexene to: 4-vinyl-1,2-epoxycyclohexane; 4-epoxyethylcyclohexene; and traces of 4-epoxyethyl-1,2-epoxycyclohexane. These epoxides are further hydrolysed by epoxide hydrolase to the corresponding diols: 4-vinylcyclohexane-1,2-diol; 4-hydroxyethylcyclohexene and possibly 4-epoxyethylcyclohexane-1,2-diol. The latter two may be further metabolised to 4-hydroxyethyl-1,2-epoxycyclohexane and tetrol 4-hydroxyethylcyclohexane-1,2-diol (9,10). Following a single oral dose of 400 mg kg^{-1} mice eliminate >95% of the dose in 24 hr, whereas rats required 48 hr to eliminate >95%. 50-60% was eliminated in the urine and 30-40% in expired air (11).

Irritancy

Irritating to the skin. Vapour or mist is irritating to the eyes, mucous membranes and upper respiratory tract (species unspecified) (12).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (13).

Other effects

Other adverse effects (human)

Keratitis, rhinitis, headache, hypotonia, leucopenia, neutrophilia, lymphocytosis and impairment of pigment and carbohydrate metabolism have been noted in exposed workers (2).

Any other adverse effects

Like other vinyl alicyclic compounds, 4-vinyl-1-cyclohexene destroys *in vitro* the hepatic microsomal cytochrome P_{450} obtained from phenobarbital treated mice (14).

Other comments

Metabolites were mutagenic in *in vitro* studies using Chinese hamster V79 cells (9,15).

Physical properties, uses, occurrence, analysis, carcinogenicity, mammalian toxicity, metabolism and mutagenicity reviewed (16,17).

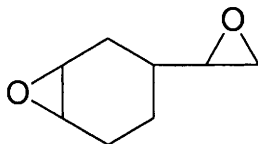
Autoignition temperature 270°C.

Formulation deterioration inhibited with 50 ppm *p*-tert-butylcatechol.

References

1. Smyth, H. F. et al *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 470.
2. Bykov, L. A. *Proc. Conf. Toxicol. Hyg. Petrochem. Ind. Prod. Moscow* 1968, 32-34 (Russ.) (*Chem. Abstr.* **75**, 40038y).
3. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-303, NIEHS, Research Triangle Park, NC, USA.
4. Giannarini, C. et al *Toxicol. Lett.* 1981, **8**, 115-121.
5. *IARC Monograph* 1987, **Suppl. 7**, 73.
6. van Duuren, B. L. in Wogan, G. N. (Ed.) *Mycotoxins in Foodstuffs* 1965, 275-285, MIT Press, Cambridge, MA, USA.
7. Collins, J. J. et al *J. Toxicol. Environ. Health* 1987, **21**(1), 507-524.
8. Smith, B. J. et al *Reprod. Toxicol.* 1991, **5**(4), 379-383.
9. Wantabe, T. et al *Xenobiotica* 1981, **11**, 333-344.
10. Gerrasi, P. G. et al in Gut, I. et al *Xenobiotics: Biotransformation and Pharmacokinetics* 1981, 205-210, Springer, Berlin, Germany.
11. Smith, B. J. et al *Toxicol. Appl. Pharmacol.* 1990, **105**(3), 364-371.
12. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **27**, 3602, Sigma-Aldrich, Milwaukee, WI, USA.
13. Zeiger, E. et al *Environ. Mutagen.* 1987, **9**(Suppl. 9), 1-109.
14. Testai, E. et al *Biochem. Biophys. Res. Commun.* 1982, **107**, 633-641.
15. Turchi, G. et al *Mutat. Res.* 1981, **83**, 419-430.
16. *IARC Monograph* 1986, **39**, 181-192.
17. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

v32 (±)-4-vinyl-1-cyclohexene diepoxide



$C_8H_{12}O_2$

Mol. Wt. 140.18

CAS Registry No. 106-87-6

Synonyms 1,2-epoxy-4-epoxyethylcyclohexane; 3-oxiranyl-7-oxabicyclo[4.1.0]heptane; 3-(epoxyethyl)-7-oxabicyclo[4.1.0]heptane; 1-epoxyethyl-3,4-epoxycyclohexane; 4-vinylcyclohexene dioxide

EINECS No. 203-437-7

RTECS No. RN 8640000

Uses Used in water-resistant adhesives, corrosion inhibitors and polymer stabilisers. Cross-linking agent and ingredient in rocket fuels and reactive diluent for epoxy resins.

Physical properties

M. Pt. -55°C **B. Pt.** 227°C **Flash point** 107.2°C **Specific gravity** 1.099 at 20°C with respect to water at 20°C

Volatility v.p. 0.1 mmHg at 20°C ; v.den. 4.86

Solubility Water: 50-100 g l⁻¹. Organic solvents: acetone, dimethyl sulfoxide, ethanol

Occupational exposure

US-TWA 0.1 ppm (0.57 mg m⁻³)

Supply classification toxic

Risk phrases Toxic by inhalation, in contact with skin and if swallowed – Possible risk of irreversible effects (R23/24/25, R40)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Do not breathe vapour – Avoid contact with the skin – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S23, S24, S45)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 2130 mg kg⁻¹ (1).

LC₅₀ (4 hr) inhalation rat 800 ppm (1).

LD₅₀ dermal rat 620 mg kg⁻¹ (2).

Sub-acute and sub-chronic data

Dermal rat (13 wk), 6.25-200 mg ml⁻¹ in acetone and dermal mouse (13 wk) 6.25-100 mg ml⁻¹ in acetone caused skin lesions. In ♀ mice follicular atrophy of the ovary occurred at high-dose levels (3).

Oral rat, mouse (13 wk), 62.5-1000 mg kg⁻¹ caused decrease in body weight. Target organs in rats were forestomach and kidney, in mice forestomach and testis (3).

Intraperitoneal mouse (30 day), 0, 100, 400, 800 mg kg⁻¹ day⁻¹ induced follicle loss in the ovary (4).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, limited evidence for carcinogenicity to animals, IARC classification group 3 (5).

National Toxicology Program tested rats and mice by painting skin. Clear evidence of carcinogenic activity demonstrated in ♂ and ♀ rats and mice (6).

Dermal rat (105 wk or 15 month) at 0, 15, 30 mg animal⁻¹ 5 × wk⁻¹ and dermal mice (105 wk or 15 month) at 0, 2.5, 5, 10 mg animal⁻¹ 5 × wk⁻¹ induced squamous cell carcinomas of the skin and ovarian neoplasms in ♀ animals.

Increased incidence of lung neoplasms were also observed (7,8).

Teratogenicity and reproductive effects

Intraperitoneal ♀ rats, mice (30 day), 10-1000 mg kg⁻¹ day⁻¹ gave an ED₅₀ (the reduction of small oocyte count to 50%) at dose levels 30-60 mg kg⁻¹ (9).

Irritancy

Dermal rabbit 545 mg open (duration unspecified) caused mild irritation (2).

Dermal rabbit 500 mg (duration unspecified) caused severe irritation (1).

Genotoxicity

In vitro mouse lymphoma L5178Y tk⁺/tk⁻ positive (10).

Other comments

Reviews on human health effects, experimental toxicology, workplace experience, epidemiology listed (11).

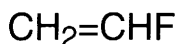
Ovarian toxicity and carcinogenicity in National Toxicology Program studies reviewed (12).

Toxicology reviewed (13).

References

1. Sax, N. I. et al *Dangerous Properties of Industrial Materials* 8th ed., 1992, Van Nostrand Reinhold, New York, NY, USA.
2. *Union Carbide Data Sheet* 1975, 28 August, Union Carbide Corp., New York, NY, USA.
3. Chhabra, R. S. *Fundam. Appl. Toxicol.* 1990, **14**(4), 745-751.
4. Smith, W. J. et al *Reprod. Toxicol.* 1991, **5**(4), 379-383.
5. *IARC Monograph* 1987, **Suppl.7**, 63.
6. *National Toxicology Program Research and Testing Division* 1992, Report No. TR-362, NIEHS, Research Triangle Park, NC, USA.
7. Chhabra, R. S. *Fundam. Appl. Toxicol.* 1990, **14**(4), 752-763.
8. Chhabra, R. S. *Report*, 1989, NTP-TR-362, PB90-219957, National Toxicology Program, Research Triangle Park, NC, USA.
9. Smith, W. J. et al *Toxicol. Appl. Pharmacol.* 1990, **105**(3), 372-381.
10. McGregor, D. B. et al *Environ. Mol. Mutagen.* 1988, **12**(1), 85-154.
11. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium.
12. Maronpot, R. R. *Environ. Health Perspect.* 1987, **73**, 125-130.
13. *J. Appl. Toxicol.* 1996, **16**(5), 465-468

v33 vinyl fluoride



$\text{C}_2\text{H}_3\text{F}$

Mol. Wt. 46.04

CAS Registry No. 75-02-5

Synonyms fluoroethylene; 1-fluoroethene; monofluoroethylene; fluoroethene

EINECS No. 200-832-6

RTECS No. YZ 7351000

Uses Manufacture of polymers. Solvent.

Physical properties

M. Pt. -160.5°C B. Pt. -72°C Volatility v.den. 1.58

Solubility Organic solvents: acetone, diethyl ether, ethanol

Occupational exposure

FR-VME 2.5 mg m^{-3} (as F)

SE-LEVL 2 mg m^{-3} (as F)

UK-LTEL 2.5 mg m^{-3} (as F)

US-TWA 1 ppm

UN No. 1860 (inhibited) HAZCHEM Code 2WE (inhibited) Conveyance classification flammable gas (inhibited)

Mammalian & avian toxicity

Sub-acute and sub-chronic data

Inhalation rat (14 wk) 2000 ppm 8 hr day $^{-1}$ 5 day wk $^{-1}$ induced pre-neoplastic hepatic foci (1).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (2).

Inhalation rat and mouse (6 hr day $^{-1}$, 5 days wk $^{-1}$ for 2 yrs) 0, 25, 250, and 2500 ppm. A decrease in body-weight gain was observed in mice and rats. An increase in the incidence of palpable masses in the mammary gland region of mice was observed. Urinary fluoride excretion increased to a plateau at 250 ppm in rats and mice. Above 25 ppm, vinyl fluoride was found to be carcinogenic to both mice and rats (3).

Metabolism and toxicokinetics

Readily absorbed via inhalation in rats and an equilibrium concentration reached in the entire animal which was 90% of that in the gas phase. Metabolism was saturable after exposure to $>140 \text{ mg m}^{-3}$ and associated with the release of fluoride into the urine (4,5).

When incubated with liver microsomes from phenobarbitone-treated rats, vinyl fluoride alkylated the prosthetic group (haem) of cytochrome P₄₅₀. The alkylated moiety has been identified as the dimethyl ester of *N*-(2-oxoethyl)protoporphyrin IX (6).

Like other halogenated C₁ and C₂ compounds that are transformed to reactive metabolites, fluoroethene causes changes in rat carbohydrate intermediary metabolism leading to increased exhalation of acetone (7).

Genotoxicity

Drosophila melanogaster sex-linked recessive lethal assay positive (8).

In vitro Chinese hamster hypoxanthine-guanine phosphoribosyl transferase locus and chromosome aberrations, with metabolic activation positive (8).

In vitro mouse bone marrow, induction of micronuclei positive (8).

No unscheduled DNA synthesis was detected in pachytene spermatocytes, no DNA single strand breaks or DNA-DNA cross-links were detected by alkaline elution of testicular DNA, and no dominant lethal mutations occurred

following inhalation exposure of σ^7 rats. The study showed that vinyl fluoride posed no risk of heritable mutations in mammals (8).

Other effects

Any other adverse effects

Acute inhalation toxicity cannot be determined due to the occurrence of asphyxia (9).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (10).

Other comments

Requirements for toxicological assessment are specified in the Federal Register (11).

Toxicology of fluorine-containing monomers reviewed (12).

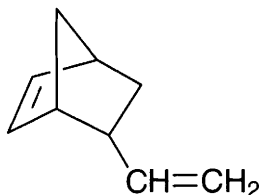
Physical properties, use, analysis, toxicity and metabolism reviewed (13).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (14).

References

1. Balt, H. M. *Arch. Toxicol.* 1981, **47**(1), 71-73.
2. *IARC Monograph* 1987, **Suppl.7**, 73.
3. Bogdanffy, M. S. et al *Fundam. Appl. Toxicol.* 1995, **26**(2), 223-238.
4. Filser, J. G. et al *Arch. Toxicol.* 1981, **47**, 279-292.
5. Dilley, J. V. et al *Toxicol. Appl. Pharmacol.* 1979, **27**, 582-590.
6. Ortiz de Montellaro, P. R. et al *Biochemistry* 1982, **21**, 1331-1339.
7. Filser, J. G. et al *Arch. Toxicol.* 1982, **49**, 107-116.
8. Bentley, K. S. et al *Environmental Mutagen Society, 23rd Annu. Sci. Meet.* 1992, *Abstr. Environ. Mol. Mutagen.* 1992, **19**(Suppl. 20), 5.
9. Clayton, J. W. *Fluorine Chem. Rev.* 1967, **1**, 197-252.
10. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
11. *Fed. Regist.* 1991, **56**(98), 23228-23232.
12. Kennedy, G. L. et al *Crit. Rev. Toxicol.* 1990, **21**(2), 149-170.
13. *IARC Monograph* 1986, **39**, 147-154.
14. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

V34 5-vinyl-2-norbornene



C₉H₁₂

Mol. Wt. 120.19

CAS Registry No. 3048-64-4

Synonyms bicyclo[2.2.1]hept-2-ene; 5-ethenylbicyclo[2.2.1]hept-2-ene; 2-vinylnorbornene

EINECS No. 221-259-8

RTECS No. RC 0350000

Uses Manufacture of polymers, mainly as an intermediate in the production of EPDM rubber.

Physical properties

M. Pt. -80°C B. Pt. 141°C Flash point 27°C Specific gravity 0.841 Volatility v.p. 6.0 mmHg at 20°C

Occupational exposure

UN No. 1993

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 4400-5700 mg kg⁻¹ (1,2).

LC_{Lo} (4 hr) inhalation rat 4000 ppm (1).

LC₅₀ (2 hr) inhalation mouse 18,000 mg m⁻³ (3).

LD₅₀ dermal rabbit 13,000 mg kg⁻¹ (1).

LD₅₀ intravenous rabbit 0.10 (♂), 0.05 (♀) mg kg⁻¹ (4).

Metabolism and toxicokinetics

May be absorbed by inhalation, ingestion or via the skin (species unspecified) (3).

Irritancy

Vapour or mist is irritating to the eyes, mucous membranes and upper respiratory tract (species unspecified) (3).

Genotoxicity

Salmonella typhimurium reverse mutation assay with and without metabolic activation negative. No significant concentration-related increase in mutation frequency found in a forward gene mutation test in CHO cells with or without metabolic activation. SCE assay, with or without metabolic activation, negative. No significant or dose-related increases in chromosomal aberrations observed in bone marrow of Sprague-Dawley rats exposed to vapour concentrations up to 336 pmm for 6 hr day⁻¹ (5).

Other effects

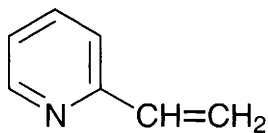
Any other adverse effects

Causes hyaline droplet nephropathy in ♂ rats (5).

References

1. *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 470.
2. Dobryira, V. V. et al *Gig. Tr. Prof. Zabol.* 1974, **18**(10), 52.
3. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3606, Sigma-Aldrich, Milwaukee, WI, USA.
4. Ballantyne, B. et al *J. Appl. Toxicol.* 1997, **17**(4), 211-221.
5. Vergnes, J. S. et al *J. Appl. Toxicol.* 1998, **18**(2), 129-142

V35 2-vinylpyridine



C₇H₇N

Mol. Wt. 105.14

CAS Registry No. 100-69-6

EINECS No. 202-879-8

RTECS No. UU 1040000

Uses Chemical intermediate for a variety of syntheses including pharmaceuticals.

Occurrence Component of tobacco smoke (1,2).

Pollutant in river waters and bottom sediments (3).

Physical properties

M. Pt. 56-57°C B. Pt. 158-159°C Flash point 42°C Specific gravity 0.973-0.976 at 20°C

Other comments

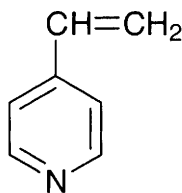
Toxicity in wastewater has been evaluated using bacteria (4).

Inhibits the germination of seeds of 17 species of common weeds (5).

References

1. Proctor, C. J. *Environ. Technol. Lett.* 1989, **10**(11), 1003-1018.
2. Eatough, D. J. *Environ. Int.* 1989, **15**(1-6), 19-28.
3. Tsukioka, T. et al *J. Chromatogr.* 1987, **396**, 319-326.
4. Farago, C. et al *Rev. Chim. (Bucharest)* 1969, **40**(2), 166-170 (Rom.) (*Chem. Abstr.* **111**, 159568y).
5. Leather, G. R. *J. Agric. Food. Chem.* 1990, **38**(3), 856-859

V36 4-vinylpyridine



C₇H₇N

Mol. Wt. 105.14

CAS Registry No. 100-43-6

Synonyms 4-ethenylpyridine; 4-VP

EINECS No. 202-852-0

RTECS No. UU 1045000

Uses Manufacturer of polymers. Organic synthesis.

Physical properties

B. Pt. 62-65°C at 15 mmHg Flash point 51°C Specific gravity 0.9800 at 20°C with respect to water at 4°C

Partition coefficient log P_{ow} 1.80 (1) Volatility v.p. 2 mmHg at 25°C

Solubility Water: 29 g l⁻¹ at 20°C. Organic solvents: chloroform, diethyl ether, ethanol

Occupational exposure

UN No. 3073 (inhibited) HAZCHEM Code 3W (inhibited) Conveyance classification toxic substance, danger of fire (flammable liquid) (inhibited)

Ecotoxicity

Invertebrate toxicity

IC₅₀ (60 hr) *Tetrahymena pyriformis* 8.9 mg l⁻¹ (1).

EC₅₀ (30 min) *Photobacterium phosphoreum* 9.8 ppm Microtox test (2).

Bioaccumulation

Estimated bioconcentration factor 1.9-6.8 indicates that environmental accumulation is unlikely (3).

Environmental fate

Abiotic removal

Reacts with photochemically produced hydroxyl radicals in the atmosphere estimated t_{1/2} 14.5 hr (4).

Estimated volatilisation t_{1/2} 12 days from model river water, 133 days from model pond water (4,5).

Adsorption and retention

Estimated K_{oc} 15-136 indicate no significant adsorption to soil and sediments (6).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, redwing blackbird 100 mg kg⁻¹ (7,8).

LC_{Lo} (2 hr) inhalation rat 2000 ppm (8).

LD₅₀ dermal guinea pig 500 mg kg⁻¹ (8).

Sensitisation

Has been reported to cause allergic respiratory and skin reactions (species unspecified) (9).

Other effects

Other adverse effects (human)

Extremely destructive to tissue of the mucous membrane and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema (9).

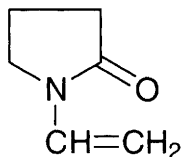
Other comments

Preparations inhibited with 0.1% w/w *tert*-butylcatechol.

References

1. *Ecotoxicol. Environ. Saf.* 1987, **13**(1), 76.
2. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
3. *EXAMS II Computer Simulation* 1987, US EPA, Athens, GA, USA.
4. Atkinson, R. et al *Chem. Rev.* 1984, **84**, 437-470.
5. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
6. Eatough, D. J. et al *Environ. Sci. Technol.* 1989, **23**, 679-687.
7. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
8. Marhold, J. V. *Průhled Průmyslové Toxikologie: Organické Latky* 1986, Prague, Czechoslovakia.
9. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3606, Sigma-Aldrich, Milwaukee, WI, USA

V37 *N*-vinyl-2-pyrrolidinone



C₆H₉NO

Mol. Wt. 111.14

CAS Registry No. 88-12-0

Synonyms 1-ethenyl-2-pyrrolidinone; vinylbutylolactam; *N*-vinylpyrrolidinone; 1-vinyl-2-pyrrolidinone; V-Pyrol

EINECS No. 201-800-4

RTECS No. UY 6107000

Uses Manufacture of polymers.

Physical properties

M. Pt. 13.5°C **B. Pt.** 148°C at 100 mmHg **Flash point** 93°C (open cup) **Specific gravity** 1.040 at 25°C with respect to water at 4°C **Volatility** v.p. 0.1 mmHg at 24°C ; v.den. 3.8

Solubility Water: miscible. Organic solvents: acetone, benzene, diethyl ether, ethanol, toluene

Occupational exposure

FR-VME 0.1 ppm

Environmental fate

Abiotic removal

Polymerises readily in the presence of oxygen (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird >100 mg kg⁻¹ (2).

LD₅₀ oral rat 1470 mg kg⁻¹ (3).

LC₅₀ inhalation rat 3200 mg m⁻³ (exposure unspecified) (3).

LD₅₀ dermal rabbit 560 mg kg⁻¹ (3).

Sub-acute and sub-chronic data

Inhalation rat (13 wk) no-observed-adverse-effect level 1 ppm; (7 wk) 5 ppm caused atrophy of olfactory epithelium and hyperplasia of nasal respiratory epithelium (4).

Inhalation rats (12 wk) ≥ 5 ppm, inhalation mice and hamsters (1 day) 45 ppm caused reduced body-weight gain.

Haematology and clinical chemistry parameters were affected and increased liver weight and liver lesions were seen in rats and mice, but not hamsters (4).

Gavage rat (12 wk) 40 mg kg⁻¹ day⁻¹ caused increased liver weight and liver lesions (4).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (polyvinyl pyrrolidone) (5).

Inhalation Sprague-Dawley rats (2 yr) 0-20 ppm 6 hr day⁻¹ 5 day wk⁻¹. Survival was unaffected but reduced body-weight gain, haemotoxicity, indications of hepatotoxicity, increased liver weight, hepatocellular carcinomas, necrosis, reparative hyperplasia, adenomas and adenocarcinomas of the nasal cavity, and squamous cell carcinomas of the larynx were seen. Only in the liver and upper respiratory tract were increased tumour incidences seen. Since *N*-vinyl-2-pyrrolidinone gives negative results in genotoxicity tests, the authors suggest that the tumours were manifestations of a non-genotoxic mechanism (6).

Metabolism and toxicokinetics

Absorbed by ingestion, inhalation and via the skin (species unspecified) (7).

Irritancy

100 mg instilled into rabbit eye caused severe irritation (exposure unspecified) (3).

Vapour or mist is irritating to the eyes, mucous membranes and upper respiratory tract. Irritating to the skin (species unspecified) (7).

Genotoxicity

Negative in *in vitro* and *in vivo* genotoxicity tests (6).

Other comments

Physical properties, uses, analysis, carcinogenicity, mammalian toxicity, metabolism and mutagenicity of polyvinyl pyrrolidone reviewed (1,8).

Autoignition temperature 360°C.

Preparations inhibited with potassium hydroxide or *N,N'*-di-*sec*-butyl-*p*-phenylenediamine.

References

1. IARC Monograph 1979, 19, 461-477.
2. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, 12, 355-382.
3. Lewis, R. J. *Sax's Dangerous Properties of Industrial Materials* 8th ed., 1989, Van Nostrand Reinhold, New York, NY, USA.
4. Klimisch, H.-J. et al *Food Chem. Toxicol.* 1997, 35(10-11), 1061-1074
5. IARC Monograph 1987, **Suppl.** 7, 73.
6. Klimisch, H.-J. et al *Food Chem. Toxicol.* 1997, 35(10-11), 1041-1060.
7. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, 2, 3606, Sigma-Aldrich, Milwaukee, WI, USA.
8. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

v38 vinyl sulfone



C₄H₆O₂S

Mol. Wt. 118.16

CAS Registry No. 77-77-0

Synonyms divinyl sulfone; 1,1'-sulfonylbisethene; TL 797

EINECS No. 201-057-6

RTECS No. KM 7175000

Uses Cross-linking agent.

Physical properties

M. Pt. -26°C B. Pt. 234°C Flash point 102°C Specific gravity 1.177

Solubility Water: miscible

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 32 mg kg⁻¹ (1).

LC_{Lo} (10 min) inhalation mouse 990 mg m⁻³ (2).

LD₅₀ dermal rabbit 22 mg kg⁻¹ (1).

LD₅₀ subcutaneous rat, mouse 14, 16 mg kg⁻¹, respectively (3).

LD₅₀ intravenous rat, mouse 11, 12 mg kg⁻¹, respectively (3).

LD₅₀ intraperitoneal rat 3 mg kg⁻¹ (4).

Metabolism and toxicokinetics

Absorbed by ingestion, inhalation and through the skin (species unspecified) (5).

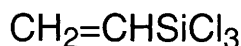
Irritancy

Dermal rabbit, 50 mg caused moderate irritation; 50 mg instilled into rabbit eye caused moderate irritation (exposure not specified) (6).

References

1. *Am. Ind. Hyg. Assoc. J.* 1962, **23**, 95.
2. *Progress Report* 1943, No. 9-4-1-9, Natl. Defence Res. Committee, Office of Scientific Res. Dev.
3. *J. Pharmacol. Exp. Ther.* 1948, **93**, 1.
4. *Toxicol. Appl. Pharmacol.* 1975, **31**, 222.
5. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3607, Sigma-Aldrich, Milwaukee, WI, USA.
6. *Union Carbide Data Sheet* 18 March 1965, Union Carbide Corp., New York, NY, USA

v39 vinyltrichlorosilane



C₂H₃Cl₃Si

Mol. Wt. 161.49

CAS Registry No. 75-94-5

Synonyms trichlorovinylsilane; trichloroethenylsilane; A150; vinylsilicon trichloride

EINECS No. 200-917-8

RTECS No. VV 6125000

Physical properties

M. Pt. -95°C B. Pt. 90.6°C Flash point 10°C Specific gravity 1.265 at 25°C with respect to water at 25°C

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1280 mg kg⁻¹ (1).

LC_{Lo} (4 hr) inhalation rat 500 ppm (2).

LD₅₀ dermal rabbit 680 mg kg⁻¹ (1).

Irritancy

Dermal rabbit 625 mg caused severe irritation (duration unspecified) (2).

50 µg instilled into rabbit eye caused severe irritation (1).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Organochlorine compounds: guide level 1 µg l⁻¹ (3).

References

1. *AMA Arch. Ind. Hyg. Occup. Med.* 1954, **10**, 61.
2. *Union Carbide Data Sheet* 19th January 1972.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

V40 vitamin A

C₂₀H₃₀O

Mol. Wt. 286.46

CAS Registry No. 11103-57-4

Synonyms Microvit A; Provitamin A; Hydrovit A; LPK; Rovimix A 500

EINECS No. 234-328-2

Uses Dietary supplement. Antixerophthalmic vitamin.

Occurrence Dietary sources include animal tissues such as liver, kidney, dairy produce, eggs and fish liver oils. Also derived from carotenes which are found in carrots, green and yellow vegetables (1).

Physical properties

M. Pt. 61-63°C **B. Pt.** distills at 120-125°C at 5 × 10⁻³ mmHg

Solubility Organic solvents: acetone, benzene, chloroform, diethyl ether, ethanol, vegetable oils

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 1500, 2000 mg kg⁻¹, respectively (2,3).

LD₅₀ intraperitoneal mouse 1500 mg kg⁻¹ (4).

Teratogenicity and reproductive effects

Oral rat, lowest toxic dose 77 mg kg⁻¹ day⁻¹ on days 8-10 of gestation, reduced foetal weight and produced behavioural effects (5).

Gavage rat, 5-10 × 10⁴ IU Vitamin A kg⁻¹ on days 8, 9, 10 or 11 of gestation. A high rate of cleft palate was induced when vitamin A was administered on day 10 of gestation (6).

Intraperitoneal rat, lowest toxic dose 30 mg kg⁻¹ on day 11 of gestation, teratogenic effects on musculoskeletal system (7).

Oral mouse, single toxic dose 75 mg kg⁻¹ day⁻¹ on days 7-11 of gestation, treatment on days 7-9 induced malformations of the head, while treatment on day 11 included bilateral forelimb reduction defects (8).

Metabolism and toxicokinetics

36-42% absorption from rat intestine into the lymphatic circulation following infusion into the jejunum.

Absorption was highest in rats at 23 months of age and lowest at 2 months of age. Vitamin A is cumulatively stored in the liver (9).

When administered to rats in excess, vitamin A levels decreased in the liver. This was explained in part by an enhanced rate of vitamin A degradation as a function of increased concentration of retinol in the liver. At high retinol concentrations, retinol metabolism via the hepatic cytosolic retinol dehydrogenase (EC 1.1.1.1) and microsomal retinol dehydrogenase and oxidase vastly exceeded the decrease in fractional recovery of vitamin A accumulation in the tissues. This rise in metabolic rate was verified by a corresponding increase in urinary polar metabolites derived from labelled retinol (10).

Vitamin A esters are hydrolysed by pancreatic enzymes to retinol, which is then absorbed (1).

Undergoes glucuronide conjugation and subsequent oxidation to retinol and retinoic acid, which are excreted in the urine and faeces (1).

Genotoxicity

In vitro Syrian hamster epithelial cells and Chinese hamster ovary cells, sister chromatid exchanges and chromosomal aberrations positive (11,12).

Other comments

1 IU equals 0.000344 mg vitamin A (1).

Vitamin A deficiency is rare in developed countries and is usually only seen in certain medical conditions, such as

biliary cirrhosis or cholestatic jaundice. Deficiency in developing countries is associated with increased risk of infections (1).

Metabolism of vitamin A reviewed (13).

Teratogenicity, immunosuppression and toxicity of vitamin A reviewed (14-16).

Action on skin and mucous membranes reviewed (17).

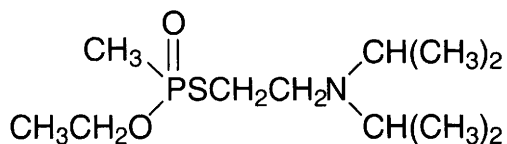
Following withdrawal of vitamin A from diet, spermatogenesis was reversibly inhibited in rats (18,19).

Effect of vitamin A in foetus and newborn reviewed (20).

References

1. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
2. *Acta Dermat. Venerol. Suppl.* 1975, **74**, 29.
3. Sporn, M. B. et al (Eds.) *The Retinoids* 1984, **2**, 287, Academic Press, New York, NY, USA.
4. Kamm, J. J. *J. Am. Acad. Dermatol.* 1982, **6**, 652.
5. *Neurobehav. Toxicol. Teratol.* 1981, **3**, 1.
6. Fujiwara, H. et al *Aichi Gakuin Daigaku Shigakkaishi* 1989, **27**(3), 629-634 (Japan.) (*Chem. Abstr* **112**, 157088p).
7. *Teratology* 1986, **33**, 1.
8. *Teratog., Carcinog., Mutagen.* 1985, **5**, 355.
9. Hollander, D. et al *Exp. Gerontol.* 1990, **25**(1), 61-65.
10. Leo, M. A. et al *J. Nutr.* 1989, **119**(7), 993-1000.
11. Mohr, U. et al *Mutat. Res.* 1991, **246**, 67-73.
12. Rosenkranz, H. S. et al *Environ. Mol. Mutagen.* 1990, **16**, 149-177.
13. Blomhoff, R. et al *Science (Washington DC)* 1990, **25**(4979), 399-404.
14. Hathcock, J. N. et al *Am. J. Clin. Nutr.* 1990, **52**(2), 183-202.
15. Underwood, B. A. *Int. J. Vitam. Nutr. Res. Suppl.* 1989, **30**, 42-55.
16. Watson, R. R. et al *Contemp. Issues Clin. Nutr.* 1988, **11**, 87-99.
17. Jarrett, A. *J. Appl. Cosmetol.* 1989, **7**(2), 33-38.
18. Bartlett, J. M. S. et al *Biol. Reprod.* 1990, **42**(4), 603-612.
19. Van Pelt, A. M. M. et al *Biol. Reprod.* 1990, **42**(4), 677-682.
20. Goradischer, R. *Dev. Pharmacol. Ther.* 1991, **15**(3-4), 166-172

V41 VX



$C_{11}H_{26}NO_2PS$

Mol. Wt. 267.37

CAS Registry No. 50782-69-9

Synonyms S-[2-[bis(1-methylethyl)amino]ethyl] O-ethyl methylphosphonothioate; MPT; Tx60; VX Vapour
RTECS No. TB 1090000

Uses Chemical warfare agent.

Physical properties

M. Pt. $\geq 51^\circ C$ **B. Pt.** $298^\circ C$ **Specific gravity** 1.0083 at $25^\circ C$ **Volatility** v.p. 7.0×10^{-4} mmHg
Solubility Water: 30 g l⁻¹

Mammalian & avian toxicity

Acute data

TD_{Lo} oral man 4 µg kg⁻¹ (1).

LD_{Lo} dermal human 86 µg kg⁻¹ (2).

LD₅₀ intraperitoneal mouse 50 µg kg⁻¹ (3).

LD₅₀ subcutaneous rat, rabbit, mouse 12, 14, 22 µg kg⁻¹, respectively (4,5,6).

Legislation

Included in Schedule 4 (Release into Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (7).

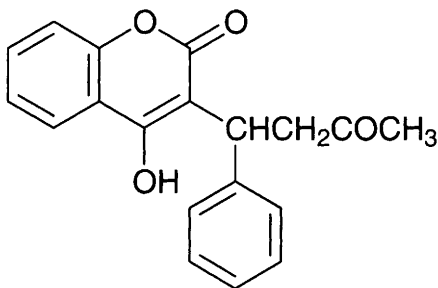
Other comments

Potent cholinesterase inhibitor.

References

1. *Toxicol. Appl. Pharmacol.* 1974, **27**, 241.
2. *WHO Technical Report* 1970, **24**, WHO, Geneva, Switzerland.
3. *WHO Technical Report* No. 39, 1970, WHO, Geneva, Switzerland.
4. *Arch. Int. Pharmacodynam. Ther.* 1983, **262**, 231.
5. *Arch. Belges Med. Soc., Hyg., Med. Trav. Med. Legale* 1984, **226**, (Suppl.).
6. *Acta Pharm. Jugoslavia* 1980, **30**, 151.
7. *S. I. No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

W1 warfarin



C₁₉H₁₆O₄

Mol. Wt. 308.33

CAS Registry No. 81-81-2

Synonyms 4-hydroxy-3-(3-oxo-1-phenylbutyl)coumarin; 4-hydroxy-3-(3-oxo-1-phenylbutyl)-2H-1-benzopyran-2-one; 3-(α-acetonylbenzyl)-4-hydroxycoumarin; coumafen; Dethmor; Kumadu; Kumatox; Katron; Rodafarin; Zoocoumarin; (±)-warfarin

EINECS No. 201-377-6

RTECS No. GN 4550000

Uses Rodenticide. Anticoagulant.

Physical properties

M. Pt. 161°C **Partition coefficient** log P_{ow} 2.52 (1) **Volatility** v.p. 67-68 × 10⁻³ mmHg at 21.5°C

Solubility Water: 17 mg l⁻¹ at 20°C. Organic solvents: acetone, dioxane, ethanol, isopropanol, methanol

Occupational exposure

DE-MAK 0.5 mg m⁻³ (inhalable fraction of aerosol)

FR-VME 0.1 mg m⁻³

UK-LTEL 0.1 mg m⁻³

UK-STEL 0.3 mg m⁻³

US-TWA 0.1 mg m⁻³

Supply classification toxic

Risk phrases May cause harm to the unborn child – Toxic: danger of serious damage to health by prolonged exposure if swallowed (R61, R48/25)

Safety phrases Restricted to professional users – Avoid exposure – obtain special instruction before use – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S53, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (24-96 hr) harlequin fish 12-17 mg l⁻¹ (2).

Threespine stickleback, steelhead trout, sockeye salmon (24 hr) 10 mg l⁻¹ static bioassay caused no loss of equilibrium or death (3).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 47.8 ppm Microtox test (4).

Bioaccumulation

Estimated bioconcentration factor 48 indicates a low potential for environmental accumulation (5).

Environmental fate

Degradation studies

Reduced by *Nocardia* and *Arthrobacter* species to the alcohol (6).

Abiotic removal

Reacts with photochemically produced hydroxyl radicals and ozone in the atmosphere, estimated t_{1/2} ~11 min (7).

Adsorption and retention

Estimated K_{oc} 560 indicates moderate adsorption to soil and sediments (5).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 2, 60 mg kg⁻¹, respectively (8,9).

LC₅₀ (duration unspecified) inhalation rat 320 mg m⁻³ (10).

LD₅₀ dermal rat 1400 mg kg⁻¹ (10).

LD_{Lo} intraperitoneal rat, subcutaneous mouse 420, 800 mg kg⁻¹, respectively (11,12).

LD_{Lo} oral human 6660 µg kg⁻¹ (8).

Sub-acute and sub-chronic data

Oral dog (3 day) 0.8 g kg⁻¹ body weight in food. On the 4th day there was a drop in haemoglobin level, and in the number of erythrocytes and thrombocytes. The number of leukocytes and juvenile granulocytes increased significantly. Following subcutaneous administration of vitamin K (10 mg kg⁻¹ body weight) recovery occurred (13).

LC₅₀ (28 day) oral mink 11.7 ppm (diet). No secondary toxicity was observed suggesting that binding and/or alteration to non- or less-toxic metabolites occurs (14).

Teratogenicity and reproductive effects

Classified as a human developmental toxicant, causing nasal hypoplasia, shortened extremities and abortion. No effects detected in rabbits and equivocal effects in mice (15).

Sprague-Dawley rats 175 µg kg⁻¹ administered as sodium salt from gestational day 8 to 22 caused 43% mortality in dams. Foetal bone osteocalcin and γ-carboxyglutamic acid levels were reduced 50 and 57%, respectively, on gestational day 22 compared with controls, which suggests that the growth plate abnormalities seen were related to the inhibition of the vitamin K-dependent proteins of the skeletal system (16).

Metabolism and toxicokinetics

Mammalian metabolites include 4-, 6-, 7- and 8-hydroxycoumarin (17,18).

Twelve healthy non-smoking adult male volunteers participated in a single-blind cross-over bioavailability study with 4 treatment phases separated by a 14 day drug-free period (2×5 mg tablets). Maximum plasma concentration 1.00 - $1.10 \mu\text{g ml}^{-1}$ was reached in ~ 1.5 to 2.5 hr (19).

Sensitisation

$1/162$ and $1/351$ subjects gave positive responses in patch tests (20,21).

Other effects

Other adverse effects (human)

Increased capillary fragility and depressed formation of prothrombin which cause haemorrhage (22).

Any other adverse effects

σ^+ oral rat single dose 0.5 , 1 , 2 mg kg^{-1} decreased insulin content of the pancreas until day 15 by 20% , 28% and 16% compared with controls. At 45 days the insulin content had almost returned to normal. Histological changes noted were hyaline degeneration in the exocrine tissue and cytoplasmic vascular degeneration and destruction of beta cells in the islets of Langerhans (23).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances of Statutory Instrument No. 472, 1991 (24).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (25).

WHO Toxicity Class Ib (26).

EPA Toxicity Class I (formation) (27).

Other comments

Pharmacology, metabolism, toxicology, mutagenicity, carcinogenicity, teratogenicity, drug safety and occupational exposure reviewed (28-36).

Environmental fate reviewed (37).

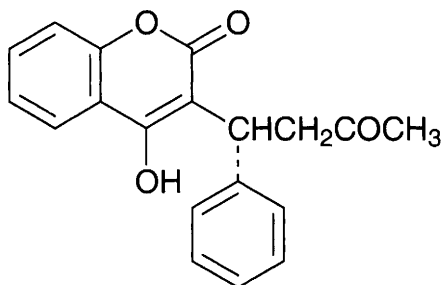
Freely soluble in alkaline aqueous solution.

References

1. Hansch, C. et al *Medchem Project Issue No. 26* 1985, Pomona College, Claremount, CA, USA.
2. Tooby, T. E. et al *Chem. Ind. (London)* 21 June 1975, 523-526.
3. MacPhee, C. et al *Fish Toxicity Screening Data* 1989, US EPA560/6-87-002 PB 87-200-275, Washington, DC, USA.
4. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
5. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
6. Davis, P. J. et al *Appl. Environ. Microbiol.* 1982, **43**, 884-890.
7. GEMS: Graphical Exposure Modeling System; Fate of Atmospheric Pollutants 1986, US EPA, Washington, DC, USA.
8. *Yakkyoku* 1977, **28**, 329.
9. *Toxicol. Appl. Pharmacol.* 1967, **11**, 327.
10. *Gig. Tr. Prof. Zabol.* 1978, **22**(7), 49.
11. *Toxicol. Appl. Pharmacol.* 1959, **1**, 156.
12. *Tr. Vses. Nauchno-Issled. Inst. Veterinarnoi Sanitarii* 1977, **58**, 122.
13. Kozak, M. et al *Folia Vet.* 1987, **31**(1), 81-88.
14. Aulerich, R. J. et al *Arch. Environ. Contam. Toxicol.* 1987, **16**(3), 357-366.
15. Jelovsek, F. R. *Obstet. Gynecol. (N.Y.)* 1989, **74**(4), 624-636.
16. Feteih, R. et al *J. Bone Miner. Res.* 1990, **5**(8), 885-894.
17. Sutcliffe, F. A. et al *Chem.-Biol. Interact.* 1990, **75**, 171.
18. Lawrence, R. F. et al *Chirality* 1990, **2**, 96.
19. Mueller, F. O. et al *SAMJ* 1988, **74**, 566-567.
20. Lisi, P. et al *Contact Dermatitis* 1986, **15**, 266-269.

21. Lisi, P. et al *Contact Dermatitis* 1987, **17**, 212-218.
22. Gosselin, R. E. et al *Clinical Toxicology of Commercial Products* 5th ed., Williams & Wilkins, Baltimore, MD, USA.
23. Ashry, M. A. et al *Proc. Zool. Soc., A. R. Egypt* 1986, **12**, 111-120.
24. S.I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
25. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of The European Communities, 2 rue Mercier, L-2985 Luxembourg.
26. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
27. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
28. Levy, G. et al *Symp. Med. Hoechst* 1986, **20**, 445-457.
29. Sutcliffe, F. A. et al *Rev. Drug Metab. Drug Interact.* 1987, **5**(4), 225-272.
30. Price, P. A. *Adv. Exp. Med. Biol.* 1987, **214**, 55-66.
31. Ioannides, C. *Hum. Toxicol.* 1988, **7**(5), 397-404.
32. Chlesara, E. et al *Rapp. ISTISAN* 1990, **90/2**(2), 219 pp. (Ital.) (*Chem. Abstr.* **14**, 253236x).
33. Esmon, C. T. *Adv. Exp. Med. Bio.* 1987, **214**, 47-54.
34. Scott, A. K. *Pharmacol. Ther.* 1989, **42**(3), 429-451.
35. Serv. Tech. Med., INRS, France *Cah. Notes Doc.* 1986, **123**, 233-236 (Fr.) (*Chem. Abstr.* **106**, 218776m).
36. Pauli, R. M. *Pathol. Immunopathol. Res.* 1988, **7**(1-2), 107-112.
37. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1991, **3**, 652-656

w2 (+)-warfarin



C₁₉H₁₆O₄

Mol. Wt. 308.33

CAS Registry No. 5543-58-8

Synonyms dextrowarfarin; *R*-(+)-warfarin; *R*-(+)-3-(α -acetylbenzyl)-4-hydroxycoumarin; (*R*)-4-hydroxy-3-(3-oxo-1-phenylbutyl)-2*H*-1-benzopyran-2-one

EINECS No. 226-908-9

Uses Anticoagulant.

Mammalian & avian toxicity

Sub-acute and sub-chronic data

Intraperitoneal rat 0.1, 0.4 or 0.8 mg kg⁻¹ day⁻¹ (total exposure unspecified) increased prothrombin times to 16.3, 21.9 and 55.1 sec, respectively. The dose of *S*-warfarin required to produce the same effects was 4 × lower (1).

Metabolism and toxicokinetics

Metabolised in rat more rapidly than laevo-warfarin in the liver, pancreas, lung, kidney, blood and intestine (2).

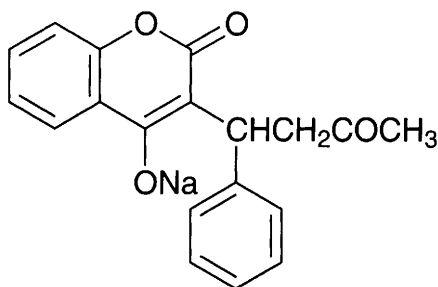
Other comments

The (*R*)-(+)-isomer has 7-fold lower rodenticide activity than the (*S*)-(-)-isomer (3).

References

1. Pratt, S. K. et al *J. Pharm. Pharmacol.* 1989, **41**(11), 743-746.
2. Syinai, I. et al *Eur. J. Drug Metab. Pharmacokinet.* 1990, **15**(2), 103-107.
3. West, B. D. et al *J. Am. Chem. Soc.* 1961, **83**, 2676

W3 warfarin sodium



$C_{19}H_{15}NaO_4$

Mol. Wt. 330.32

CAS Registry No. 129-06-6

Synonyms 3-(α -acetylbenzyl)-4-hydroxycoumarin sodium salt; Athrombin; Coumadin sodium; Panwarfin; Prothrombin; Tintorane; Warcounin; Warfilone

EINECS No. 204-929-4

RTECS No. GN 4725000

Uses Anticoagulant.

Physical properties

Solubility Water: miscible. Organic solvents: ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 8.7 mg kg⁻¹ (1).

LD₅₀ oral mouse 370 mg kg⁻¹ (2).

LD₅₀ intravenous rat, mouse 25, 160 mg kg⁻¹, respectively (3).

Teratogenicity and reproductive effects

Oral woman, lowest toxic dose 12 mg kg⁻¹ intermittently from wk 1-35 of pregnancy, parameters investigated musculoskeletal, craniofacial and cardiovascular teratogenic effects (4).

Parenteral rat (route unspecified) lowest toxic dose 2500 mg kg⁻¹ day⁻¹ on days 7-21 of gestation, parameters investigated post-implantation mortality and foetotoxicity (5).

Other effects

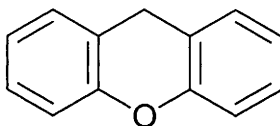
Any other adverse effects

The *in vitro* effect of warfarin sodium on nucleic acid synthesis in L1210 leukaemic cells and Walker 256 carcinosarcoma cells was studied. The incorporation of thymidine and uridine into DNA and RNA in L1210 cells was moderately inhibited, but only at very high concentrations, and no inhibition was seen in treated Walker tumour cells. The survival of L1210-bearing mice was not affected by the treatment. The compound had no *in vivo* antitumour activity against mouse L1210 activity or rat Walker 256 carcinosarcoma (6).

References

1. Baek, N. et al *Pharmacol. Res. Commun.* 1978, **10**, 445.
2. Hagen, E. C. et al *J. Am. Pharm. Soc.* 1953, **42**, 379.
3. Irvings Sunshine (Ed.) *Handbook of Analytical Toxicology* 1969, 123, Chemical Rubber Co. Cleveland, OH, USA.
4. *Am. J. Diseases Children* 1975, **129**, 360.
5. *Teratology* 1986, **33**, 86C.
6. Chang, J. C. et al *Oncology* 1973, **28**(3), 232-237

X1 xanthene



$C_{13}H_{10}O$

Mol. Wt. 182.22

CAS Registry No. 92-83-1

Synonyms 10H-9-oxaanthracene; 9H-xanthene

EINECS No. 202-194-4

RTECS No. ZD 5520000

Uses Organic synthesis. Production of xanthene dyes.

Occurrence In coal tar pitch.

Physical properties

M. Pt. 101-102°C B. Pt. 310-312°C Partition coefficient $\log P_{ow}$ 4.23 (1)

Solubility Organic solvents: benzene, carbon tetrachloride, chloroform, diethyl ether, ethanol

Ecotoxicity

Invertebrate toxicity

Xanthene was not toxic at saturation to *Tetrahymena pyriformis* in the dark and was not phototoxic after illumination with UVb for 1000 minutes (2).

Environmental fate

Degradation studies

Degraded by the white rot fungus *Phanerochaete chrysosporium* (3).

Mammalian & avian toxicity

Acute data

LD₅₀ subcutaneous mouse 690 mg kg⁻¹ (4).

Metabolism and toxicokinetics

May be absorbed by ingestion, inhalation or via the skin (species unspecified) (5).

Sensitisation

Has been reported to cause allergic respiratory and skin reactions (species unspecified) (5).

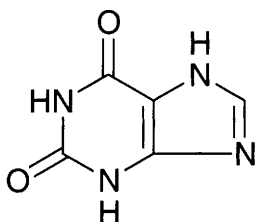
Legislation

The $\log P_{ow}$ value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (6).

References

1. Camilleri, P. et al *J. Chem. Soc. Perkin Trans. II* 1988, 1699-1707.
2. Sinks, G. D. et al *Bull. Environ. Contam. Toxicol.* 1997, **59**(1), 1-8.
3. Bumpus, J. A. *Appl. Environ. Microbiol.* 1989, **55**(1), 154-158.
4. *Arzneim.-Forsch.* 1958, **8**, 107.
5. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3617, Sigma-Aldrich, Milwaukee, WI, USA.
6. 1967 Directive on Classification, Packaging and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK

x2 xanthine



$C_5H_4N_4O_2$

Mol. Wt. 152.11

CAS Registry No. 69-89-6

Synonyms 3,7-dihydro-1*H*-purine-2,6-dione; 2,6-dioxopurine; isoxanthine; pseudoxanthine; purine-2,6-diol; 9*H*-purine-2,6-diol; 2,6(1,3)-purinedione; purine-2,6-1*H*,3*H*-dione; Xan; Xanthic oxide

EINECS No. 200-718-6

RTECS No. ZD 7700000

Uses In photographic emulsions. Central nervous system stimulant.

Occurrence Derivative of caffeine. Occurs in animal organs, yeast, potatoes, coffee beans and tea. Isolated from urinary bladder stones (1).

Physical properties

M. Pt. Decomp. on heating without melting (1) **Partition coefficient** $\log P_{ow}$ -0.99 (calc.) (2)

Solubility Water: 69 mg l⁻¹ at 16°C. Organic solvents: ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal mouse 500 mg kg⁻¹ (3).

Metabolism and toxicokinetics

Absorbed in uric acid form by isolated perfused lower intestine of the chicken (4).

Genotoxicity

Escherichia coli WP2s (λ) Microscreen assay without metabolic activation negative (5).

In vitro mouse lymphoma L5178Y cells, tk⁺/tk⁻ forward mutation assay negative (6).

Induced meiotic reductions in root tips of *Pterotheca falconeri* (7).

Other comments

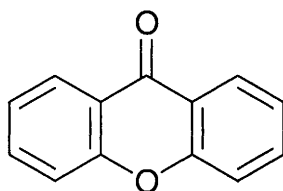
Toxicity of xanthine derivatives reviewed (8,9).

Derivatives exhibit lipolytic activity and inhibit c-AMP phosphodiesterase (10).

References

1. *The Merck Index* 12th ed., 1996, Merck & Co., Inc., Whitehouse Station, NJ, USA.
2. Verschueren, K. *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, 1188, Van Nostrand Reinhold, New York, NY, USA.
3. *NTIS Report No. AD277-689* Natl. Tech. Inf. Ser., Springfield, VA, USA.
4. Karasawa, Y. et al *Comp. Biochem. Physiol., A: Comp. Physiol.* 1991, **100A**(1), 227-230.
5. Rossman, T. G. et al *Mutat. Res.* 1991, **260**, 349-367.
6. Wengenheim, J. et al *Mutagenesis* 1988, **3**(3), 193-205.
7. Mehra, P. N. et al *Cytologia* 1986, **51**(3), 439-448.
8. Stavric, B. et al *Food Chem. Toxicol.* 1988, **26**(8), 725-733.
9. Stavric, B. et al *Food Chem. Toxicol.* 1988, **26**(7), 645-662.
10. *Mol. Pharmacol.* 1970, **6**, 597

x3 xanthone



C₁₃H₈O₂

Mol. Wt. 196.21

CAS Registry No. 90-47-1

Synonyms dibenzo- γ -pyrone; Genicide; 9-oxoxanthene; diphenylene ketone oxide; 9H-xanthen-9-one; 9-xanthenone; xanthenone; 9H-xanthen-9-one

EINECS No. 201-997-7

RTECS No. ZD 5711000

Uses Polymerisation catalyst. Solvent. Ovicide for moths. In preparation of xanthydrol.

Physical properties

M. Pt. 174-176°C B. Pt. 349-350°C at 730 mmHg

Solubility Water: slightly soluble in hot water. Organic solvents: benzene, chloroform, diethyl ether, ethanol, ligroin, light petroleum, toluene, xylene

Ecotoxicity .

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 7.5 ppm Microtox test (1).

Environmental fate

Degradation studies

Utilised by an *Arthrobacter* species (strain GFB100) as sole carbon source. An early catabolic intermediate was 3,4-dihydroxyxanthone (2).

Mammalian & avian toxicity

Acute data

LD_{Lo} oral rat > 500 mg kg⁻¹ (3).

LD₅₀ intravenous mouse 180 mg kg⁻¹ (4).

Metabolism and toxicokinetics

May be absorbed by ingestion, inhalation or via the skin (species unspecified) (5).

Sensitisation

Reported to cause allergic respiratory and skin reactions (species unspecified) (5).

Legislation

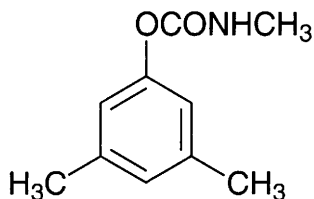
Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (6).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (7).

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
2. Tomasek, P. H. et al *J. Bacteriol.* 1986, **167**(3), 818-837.
3. National Academy of Science *Review* 1953, 5, 25, National Research Council, Chemical-Biological Coordination Center.
4. Report NX#01611, US Army Armament Res. Dev. Command, Chemical Systems Lab., Aberdeen Proving Ground, MD, USA.
5. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3618, Sigma-Aldrich, Milwaukee, WI, USA.
6. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
7. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

x4 XMC



C₁₀H₁₃NO₂

Mol. Wt. 179.22

CAS Registry No. 2655-14-3

Synonyms 3,5-xylyl methylcarbamate; Bosban; 3,5-dimethylphenyl methylcarbamate; DRC 3340; H-69; Machal; 3,5-XMC; 3,5-xylenyl N-methylcarbamate

RTECS No. FC 8925000

Uses Insecticide.

Physical properties

M. Pt. 99°C **Specific gravity** 0.54 **Partition coefficient** log P_{ow} 2.23 (1)

Solubility Water: 470 mg l⁻¹ at 20°C. Organic solvents: acetone, benzene, cyclohexanone, ethanol, ethyl acetate

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed (R22)

Safety phrases Keep out of reach of children (if sold to general public) (S2)

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) carp >40 mg l⁻¹ (2).

Invertebrate toxicity

Low toxicity to bees (3).

Bioaccumulation

Bioconcentration factor for crayfish, snail (*Physa* sp.) and catfish 100-550 (4).

Bioconcentration factor for the alga, *Oedogonium cardiacum*, and duckweed, *Lemna minor*, 2300-3050 (4).

Environmental fate

Abiotic removal

Hydrolysis t_{1/2} 13 days in alkaline soils yields 3,5-xyleneol and *N*-methylcarbamic acid (2,5).

Reacts with photochemically produced hydroxyl radicals in the atmosphere, estimated t_{1/2} 5.6 hr (6).

Estimated volatilisation t_{1/2} 1000 days from model river water (7).

Adsorption and retention

Estimated K_{oc} 390 indicates moderate adsorption to soil and sediments, although actual adsorption to soil is stronger than this value suggests (7,8).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwinged blackbird, mouse, rabbit, rat 75, 280, 445, 540 mg kg⁻¹, respectively (2,9-11).

Sub-acute and sub-chronic data

Oral rat (90 day) no-adverse-effect level 230 mg kg⁻¹ diet day⁻¹ (2).

Other effects

Any other adverse effects

Cholinesterase inhibitor (3).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (12).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (13).

WHO Toxicity Class III (14).

EPA Toxicity Class III (3).

ADI 0.0034 mg kg⁻¹ body weight (3).

Other comments

In insects, metabolism mainly involves hydroxylation of the benzene ring and the ring methyl substituents (2).

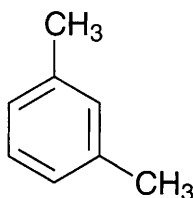
Acute toxicity is potentiated by malathion (15).

References

1. Hansch, C. et al *Medchem. Project Issue No. 26* 1985, Pomona College, Claremont, CA, USA.
2. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
3. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
4. Kanazowa, J. et al *J. Agric. Food Chem.* 1975, **23**, 760-763.
5. Passemia, L. et al *J. Environ. Sci. Health* 1989, **824**, 117-129.
6. Atkinson, R. *Int. J. Chem. Kinet.* 1987, **19**, 799-828.
7. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.

8. Kazaro, H. et al *J. Agric. Food Chem.* 1972, **20** 975-979.
9. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 335-382.
10. *Spec. Publ. Entomol. Soc. Am.* 1978, **78-1**, 56.
11. *Oyo Yakuri* 1969, **3**, 741.
12. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
13. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
14. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
15. Takahashi, N. et al *Fundam. Appl. Toxicol.* 1987, **8**(3), 415-422

x5 *m*-xylene



C₈H₁₀

Mol. Wt. 106.17

CAS Registry No. 108-38-3

Synonyms *m*-dimethylbenzene; 1,3-dimethylbenzene; *m*-methyltoluene; 3-methyltoluene; 1,3-xylene; *m*-xylol

EINECS No. 203-576-3

RTECS No. ZE 2275000

Uses Manufacture of isophthalic acid for polyester resins. Manufacture of dyestuffs and insecticides.

Occurrence Aroma component in plants and cooked meat and fish.

In fossil fuels. Residues have been detected in natural and drinking waters, sediment and in air samples (1).

Physical properties

M. Pt. -47.4°C **B. Pt.** 138-139°C **Flash point** 25°C **Specific gravity** 0.864 at 20°C with respect to water at 4°C **Partition coefficient** log *P*_{ow} 3.20 **Volatility** v.p. 10 mmHg at 28.3°C ; v.den. 3.66

Solubility Water: insoluble. Organic solvents: acetone, benzene, diethyl ether, ethanol

Occupational exposure

DE-MAK 100 ppm (440 mg m⁻³)

JP-OEL 100 ppm (430 mg m⁻³)

UK-LTEL 100 ppm (441 mg m⁻³)

UK-STEL 150 ppm (662 mg m⁻³)

US-TWA 100 ppm (434 mg m⁻³)

US-STEL 150 ppm (651 mg m⁻³)

UN No. 1307 **HAZCHEM Code** 3⁺ (flash point ≥23°C, ≤61°C, initial boiling point >35°C) **HAZCHEM Code** 3⁻ (flash point <23°C, initial boiling point >35°C) **Conveyance classification** flammable liquid

Supply classification harmful

Risk phrases Flammable – Harmful by inhalation and in contact with skin – Irritating to the skin (R10, R20/21, R38)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with the eyes (S2, S25)

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) goldfish 16 mg l⁻¹ (2).

LC₅₀ (96 hr) bass 9.2 mg l⁻¹ (3).

LC₅₀ (14 day) guppy 38 mg l⁻¹ (4).

Invertebrate toxicity

LC₅₀ (96 hr) *Crangon franciscorum* 3.7 mg l⁻¹ (3).

EC₅₀ (48 hr) *Daphnia magna* 11 mg l⁻¹ (5).

Bioaccumulation

Bioconcentration factor 23 for eels; 6.0 for clams (6,7).

Environmental fate

Degradation studies

Completely degraded in 3 wk under anaerobic conditions in a 21.5 cm continuous flow aquifer column inoculated with acclimated denitrifying bacteria (8).

Abiotic removal

Reacts with photochemically produced hydroxyl radicals in the atmosphere, estimated $t_{1/2}$ 1 hr in summer, 10 hr in winter (9).

Has a higher photochemical reactivity than the other xylene isomers under smog conditions; loss rates 9% to 42% per kg. Photooxidation products identified include glyoxal and methylglyoxal (1,10).

Estimated volatilisation $t_{1/2}$ ~3 hr from model river water; 135 hr from model pond water (11).

Adsorption and retention

Batch equilibrium measurements with soil from 3 aquifers gave K_{oc} 166; which indicates low to moderate adsorption to soil and sediments (12).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 5000 mg kg⁻¹ (13).

LC_{Lo} (4 hr) inhalation rat 8000 ppm (14).

LD₅₀ dermal rabbit 14 g kg⁻¹ (14).

LD₅₀ intraperitoneal mouse 1700 mg kg⁻¹ (15).

Sub-acute and sub-chronic data

Inhalation rats 200, 1700 or 3200 mg m⁻³ 6 hr day⁻¹ 5 day wk⁻¹ for 2 wk caused changes in the activities of brain enzymes (NADPH- diaphorase, azoreductase and superoxide dismutase) which was reversible 2 wk after cessation of exposure (16).

Inhalation rats 1700 mg m⁻³ for 6 hr day⁻¹ 5 day wk⁻¹ for 2 wk caused an increase in serum liver enzyme activities indicating liver damage (17).

Gavage rats 150, 750 or 1500 mg kg⁻¹ day⁻¹ for 60 days, and 1000 or 2000 mg kg⁻¹ day⁻¹ for 10 days caused enlarged liver and kidneys (18).

Teratogenicity and reproductive effects

Oral mouse, lowest toxic dose 30 mg kg⁻¹ day⁻¹ on days 6-15 of gestation reduced litter size (19).

Inhalation rabbit, lowest toxic concentration 500 mg m⁻³ 24 hr day⁻¹ on days 7-20 of gestation induced post implantation mortality, foetotoxic and musculoskeletal teratogenic effects (20).

Metabolism and toxicokinetics

Following inhalation exposure of rats to 200, 1700 or 3200 mg m⁻³ 6 day⁻¹ 5 day wk⁻¹ for 2 wk xylene, concentrations in the brain and perirenal fat increased during wk 2 (16).

Vapour and liquid are absorbed through human skin (21,22).

In humans, eliminated via the urine and in expired air, $t_{1/2}$ 1 hr for initial rapid phase, and ~20 hr for a slow phase. >70% was excreted via the urine as metabolites and ~5% was exhaled unchanged (23,24).

Irritancy

Dermal rabbit (24 hr) 10 µg (open) caused severe irritation (14).

5 mg instilled into rabbit eye for 24 hr caused severe irritation (25).

Genotoxicity

Salmonella typhimurium Ames mutagenicity assay negative (details not given) (26).

Drosophila melanogaster sex-linked recessive lethal assay negative (27).

In vitro Chinese hamster ovary cells, chromosomal aberrations weakly positive, sister chromatid exchanges negative (metabolic activation unspecified) (26).

In vivo mouse bone marrow cells, induction of micronuclei negative (15).

Other effects

Other adverse effects (human)

Inhalation human, lowest toxic concentration 420 mg m⁻³ 6 hr day⁻¹ for 6 days, effects to central nervous system (28).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (28).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (29).

Physical properties, uses, occurrence, analysis, carcinogenicity, mammalian toxicity, metabolism and genotoxicity of xylenes reviewed (30,31).

Other comments

NIOSH has designated xylene an ototoxin. It can cause hearing loss, ringing in the ears or total deafness and its toxicity can be exacerbated by combined exposure with noise (32).

Environmental fate reviewed (1).

Environmental health criteria reviewed (33).

WHO guideline value for total xylenes in drinking water 500 µg l⁻¹ (34).

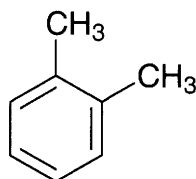
Autoignition temperature 530 °C.

References

1. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1991 **2**, 516-525, Lewis Publ., Chelsea, MI, USA.
2. *Shell Industrie Chemication Gids* 1975, Shell Chemie 's-Gravenhage, Netherlands.
3. Verschuere, K. *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, 1191-1192, Van Nostrand Reinhold, New York, NY, USA.
4. Koenemann, W. H. *Quantitative Structure-Activity Relationships for Kinetics and Toxicity of Aromatic Pollutants and their Mixtures to Fish* 1979, Univ. of Utrecht, Netherlands.
5. Vighi, M. et al *Chemosphere* 1987, **16**(5), 1043-1051.
6. Ogata, M. et al *Water Res.* 1970, **12**, 1041-1044.
7. Nures, P. et al *Bull. Environ. Contam. Toxicol.* 1979, **21**, 719.
8. Zeyer, Y. et al *Appl. Environ. Microbiol.* 1986, **52**, 944-947.
9. Ravishankara, A. R. et al *Int. J. Chem. Kinet.* 1978, **10**, 783-804.
10. Tuazon, E. C. et al *Environ. Sci. Technol.* 1986, **20**, 383-387.
11. Lyman, W. K. et al *Handbook of Chemical Property Estimation Method Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
12. Abdul, A. S. et al *Haz. Waste Haz. Mat.* 1987, **4**, 211-221.
13. *Gekkan Yahiyi* 1980, **22**, 883.
14. Smyth, H. F. et al *Am. Ind. Hyg. Assoc. J.* 1962, **23**, 95.
15. Mohtashamipur, E. et al *Arch. Toxicol.* 1985, **58**, 106-109.
16. Sardainen, K. et al *Arch. Toxicol.* 1980, **45**, 117-122.
17. Eloveara, E. *Xenobiotica* 1982, **12**, 345-352.

18. Condie, L. W. et al *Drug Chem. Toxicol.* 1988, **11**(4), 329-354.
19. *Soc. Toxicol. Ann. Meet.* 1980, **19**, Abstract 22.
20. Ungvary, G. et al *Arch. Toxicol.* 1985, **Suppl. 8**, 425-430.
21. Ruehimaki, V. et al *Scand. J. Work Environ. Health* 1978, **4**, 73-85.
22. Ergstroem, J. et al *Int. Arch. Occup. Environ. Health* 1977, **39**, 181-189.
23. Ergstroem, J. et al *Int. Arch. Occup. Environ. Health* 1984, **54**, 355-364.
24. Ruehimaki, V. et al *Xylene (Swed.) (Arbete och Halsa 1997:35)* 1979, Novellie Export Group for Criteria Documents.
25. Marhold, J. V. *Prehled Prumyslove Toxikologie: Organicke Latky* 1986, Prague, Czechoslovakia.
26. Rosenkranz, H. S. et al *Mutagenesis* 1990, **5**(6), 559-571.
27. Donner, M. et al *Mutat. Res.* 1980, **74**, 171-172.
28. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
29. 1967 *Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
30. *IARC Monograph* 1989, **47**, 125-136.
31. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium.
32. *Chem. Health Saf.* 1997, **4**(2), 29.
33. *Environmental Health Criteria* No. 190 1997, WHO/IPCS, Geneva, Switzerland.
34. *Guidelines for Drinking Water Quality* 2nd ed., 1993, 1, WHO, Geneva, Switzerland

x6 o-xylene



C₈H₁₀

Mol. Wt. 106.17

CAS Registry No. 95-47-6

Synonyms o-dimethylbenzene; 1,2-dimethylbenzene; o-methyltoluene; 2-methyltoluene; 1,2-xylene; o-xylol

EINECS No. 202-422-2

RTECS No. ZE 2450000

Uses Solvent. Manufacture of phthalic anhydride. Manufacture of dyestuffs, pharmaceuticals and insecticides.

Occurrence Aroma component of plants and cooked meat and fish.

In fossil fuels. Residues have been detected in natural waters and air samples (1).

Physical properties

M. Pt. -25 to -23°C **B. Pt.** 143-145°C **Flash point** 32°C **Specific gravity** 0.880 at 20°C with respect to water at 4°C **Partition coefficient** log P_{ow} 3.12 **Volatility** v.p. 6.8 mmHg at 25°C ; v.den. 3.7

Solubility Water: insoluble. Organic solvents: acetone, benzene, diethyl ether, ethanol

Occupational exposure

DE-MAK 100 ppm (440 mg m⁻³)

JP-OEL 100 ppm (430 mg m⁻³)

UK-LTEL 100 ppm (441 mg m⁻³)

US-TWA 100 ppm (434 mg m⁻³)

UK-STEL 150 ppm (662 mg m⁻³)

US-STEL 150 ppm (651 mg m⁻³)

UN No. 1307 HAZCHEM Code 3M (flash point $\geq 23^{\circ}\text{C}$, $\leq 61^{\circ}\text{C}$, initial boiling point $> 35^{\circ}\text{C}$) HAZCHEM Code 3ME (flash point $< 23^{\circ}\text{C}$, initial boiling point $> 35^{\circ}\text{C}$) Conveyance classification flammable liquid
Supply classification harmful
Risk phrases Flammable – Harmful by inhalation and in contact with skin – Irritating to the skin (R10, R20/21, R38)
Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with the eyes (S2, S25)

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) goldfish 13 mg l⁻¹ (2).
LC₅₀ (96 hr) rainbow trout, fathead minnow, goldfish, bass 11-42 mg l⁻¹ (3,4).
LC₅₀ (7 day) guppy 35 mg l⁻¹ (5).

Invertebrate toxicity

EC₅₀ (15 min) *Photobacterium phosphoreum* 9.25 ppm Microtox test (6).
EC₅₀ (48 hr) *Daphnia magna* 8.5 mg l⁻¹ (7).

Bioaccumulation

Bioconcentration factor eels 23; bioconcentration factor clams 5.5 (8,9).

Environmental fate

Degradation studies

Degraded under anaerobic conditions, but only under denitrifying conditions and only after the removal of other xylene isomers (10).
ThOD 3.125 (11).

Abiotic removal

Reacts with photochemically produced hydroxyl radicals in the atmosphere, estimated $t_{1/2}$ ~2 hr in summer, 15 hr in winter (12).
Photooxidation products identified include glyoxal, methylglyoxal and biacetyl (13).
Estimated volatilisation $t_{1/2}$ ~3 hr from model river water, 125 hr from model pond water (14).

Adsorption and retention

Reported K_{oc} 48 to 68 indicate low to moderate adsorption to soil and sediments (15).

Mammalian & avian toxicity

Acute data

LD_{Lo} oral rat 5000 mg kg⁻¹ (16).
LC_{Lo} (4 hr) inhalation human 8000 ppm (17).
LC_{Lo} (2 hr) inhalation mouse 2000 ppm (18).
LD₅₀ intraperitoneal mouse 1400 mg kg⁻¹ (19).

Sub-acute and sub-chronic data

Inhalation rats, guinea pigs, monkeys, dogs 3400 mg m⁻³ 8 hr day⁻¹ 5 day wk⁻¹ for 6 wk, or 340 mg m⁻³ continuously for 90 days caused no significant toxicity, or changes in body weight or in haematological parameters (20).
Inhalation rats 15,000 mg m⁻³ 8 hr day⁻¹ for 1-6 wk. Slight decreases in body-weight gain and increased liver weight were observed in both groups (21).
Gavage rats 150, 750 or 1500 mg kg⁻¹ day⁻¹ for 60 days, or 250, 1000 or 2000 mg kg⁻¹ day⁻¹ for 10 days caused enlarged liver and kidneys (22).

Teratogenicity and reproductive effects

Inhalation rat, lowest toxic concentration 1300-3000 mg m⁻³ 24 hr day⁻¹ on days 7-14 of gestation caused foetotoxic and musculoskeletal teratogenic effects (23).
Intraperitoneal ♂ rat, lowest toxic dose 500 mg kg⁻¹ 2 days prior to mating caused spermatogenic effects (24).

Genotoxicity

Salmonella typhimurium Ames mutagenicity assay negative (details unspecified) (25).

In vitro Chinese hamster ovary cells, chromosomal aberrations negative, sister chromatid exchanges positive (25).

Drosophila melanogaster sex-linked recessive lethal assay negative (26).

In vivo rat, sperm abnormality positive at 24-30°C, negative at 20-24°C. Interpreted as a synergistic affect with temperature (24).

In vivo mouse bone marrow cells, induction of micronuclei negative (19).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (27).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (28).

Other comments

NIOSH has designated xylene an ototoxin. It can cause hearing loss, ringing in the ears or total deafness and its toxicity can be exacerbated by combined exposure with noise (29).

Environmental fate reviewed (1).

Environmental health criteria reviewed (30).

WHO guideline value for total xylenes in drinking water 500 $\mu\text{g l}^{-1}$ (31).

Physical properties, uses, occurrence, analysis, carcinogenicity, mammalian toxicity, metabolism and genotoxicity of xylenes reviewed (32,33).

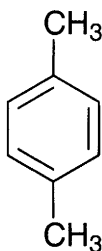
Autoignition temperature 464°C.

References

1. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1991, 2, 505-515, Lewis Publ., Chelsea, MI, USA.
2. *Shell Industrie Chemicalien Gids* 1975, Shell Chemie, s'Gravenhage, Netherlands.
3. Grenimann, G. et al *Water Res.* 1976, 10, 165-169.
4. Walsh, D. F. et al *Report No. REC-ERC-77-11* 1977, Engineering and Research Center, Bureau of Reclamation, Denver, CO, USA.
5. Koenemann, W. H. *Quantitative Structure-Activity Relationships for Kinetics and Toxicity of Aquatic Pollutants and Their Mixtures in Fish* 1979, Univ. Utrecht, Netherlands.
6. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, 26(3), 361-431.
7. Vighi, M. et al *Chemosphere* 1987, 16(5), 1043-1051.
8. Nunes, P. et al *Bull. Environ. Contam. Toxicol.* 1979, 21, 719.
9. Ogata, M. et al *Water Res.* 1978, 12, 1041-1044.
10. Meinck, F. et al *Les Eaux Residuaire Industrielle* 1970.
11. Kuhn, E. P. et al *Environ. Sci. Technol.* 1985, 19, 961-968.
12. Ravishankara, A. R. et al *Int. J. Chem. Kinet.* 1978, 10, 783-804.
13. Tuazan, E. C. et al *Environ. Sci. Technol.* 1986, 20, 383-387.
14. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
15. Nathurani, J. S. et al *Chemosphere* 1977, 6, 157-162.
16. *Gekkan Yakuji* 1980, 22, 883.
17. Smyth, H. F. et al *Am. Ind. Hyg. Assoc. J.* 1962, 23, 95.
18. *J. Pathol. Bacteriol.* 1938, 46, 95.
19. Mohtashampur, E. et al *Arch. Toxicol.* 1985, 58, 106-109.
20. Jenkins, L. J. et al *Toxicol. Appl. Pharmacol.* 1970, 16, 818-823.
21. T'atrai, E. et al *Acta Med. Acad. Sci. Hung.* 1980, 37, 211-216.
22. Condie, L. W. et al *Drug Chem. Toxicol.* 1988, 11(4), 329-354.
23. *Toxicology* 1980, 18, 61.
24. Washington, W. J. et al *Arch. Androl.* 1983, 11, 233-237.
25. Rosenkranz, H. S. et al *Mutagenesis* 1990, 5(6), 559-571.
26. Donner, M. et al *Mutat. Res.* 1980, 74, 171-172.

27. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
28. 1967 *Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
29. *Chem. Health Saf.* 1997, 4(2), 29.
30. *Environmental Health Criteria* No. 190: *Xylenes* 1997, WHO/IPCS, Geneva, Switzerland.
31. *Guidelines for Drinking Water Quality* 2nd ed., 1993, 1, WHO, Geneva, Switzerland.
32. *IARC Monograph* 1989, 47, 125-156.
33. *ECETOC Technical Report* No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

x7 **p-xylene**



C₈H₁₀

Mol. Wt. 106.17

CAS Registry No. 106-42-3

Synonyms 1,4-dimethylbenzene; *p*-dimethylbenzene; *p*-methyltoluene; 4-methyltoluene; 1,4-xylene; *p*-xylol; Chroman; Scintillar

EINECS No. 203-396-5

RTECS No. ZE 2625000

Uses Manufacture of terephthalic acid and dimethylterephthalate. Manufacture of polyester resins and fibres. Solvent. Manufacture of pesticides and pharmaceuticals.

Occurrence Aroma component of plants and cooked meat and fish.

In fossil fuels. Residues have been detected in natural waters, drinking water, sediments and air samples (1).

Physical properties

M. Pt. 12-13°C **B. Pt.** 138°C **Flash point** 27°C **Specific gravity** 0.8611 at 20°C with respect to water at 4°C

Partition coefficient log *P*_{ow} 3.15 **Volatility** v.p. 10 mmHg at 27.3°C ; v.den. 3.66

Solubility Water: insoluble. Organic solvents: acetone, benzene, diethyl ether, ethanol

Occupational exposure

DE-MAK 100 ppm (440 mg m⁻³)

JP-OEL 100 ppm (430 mg m⁻³)

UK-LTEL 100 ppm (441 mg m⁻³)

UK-STEL 150 ppm (662 mg m⁻³)

US-TWA 100 ppm (434 mg m⁻³)

US-STEL 150 ppm (651 mg m⁻³)

UN No. 1307 **HAZCHEM Code** 3⁺ (flash point ≥23°C, ≤61°C, initial boiling point >35°C) **HAZCHEM Code** 3⁻ (flash point <23°C, initial boiling point >35°C) **Conveyance classification** flammable liquid

Supply classification harmful

Risk phrases Flammable – Harmful by inhalation and in contact with skin – Irritating to the skin (R10, R20/21, R38)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with the eyes (S2, S25)

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) goldfish 18 mg l⁻¹ (2).

LC₅₀ (96 hr) fathead minnow, bluegill sunfish, goldfish, guppy 24-37 mg l⁻¹ (3).

LC₅₀ (7 day) guppy 35 mg l⁻¹ (4).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 5.7 ppm Microtox test (5).

EC₅₀ (48 hr) *Daphnia magna* 3.2 mg l⁻¹ (6).

LC₅₀ (96 hr) *Crangon franciscorum* 2.0 mg l⁻¹ (7).

Bioaccumulation

Bioconcentration factor for eels 23 (8).

Environmental fate

Degradation studies

Readily biodegraded in shallow groundwater in a sand aquifer. As the available oxygen was consumed, the rate of degradation decreased (9).

Abiotic removal

Reacts with photochemically produced hydroxyl radicals in the atmosphere, estimated $t_{1/2}$ ~2 hr in summer, 18 hr in winter (10).

Moderately reactive under photochemical smog conditions; reported loss rates of 4-25% hr⁻¹, which are typical of the reaction with hydroxyl radicals (1,11).

Estimated volatilisation $t_{1/2}$ ~3 hr for model river water and 135 hr from model pond water (12).

Adsorption and retention

Batch equilibrium measurements from soil in 3 aquifers gave a K_{oc} of 204 (13).

K_{oc} 25.4 for surface sediment in the Tarron estuary (14).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 5000 mg kg⁻¹ (15).

LC₅₀ (4 hr) inhalation rat 4500 ppm (16).

LD₅₀ intraperitoneal rat, mouse 2100, 3800 mg kg⁻¹, respectively (16,17).

Sub-acute and sub-chronic data

Inhalation rat 6500 mg m⁻³ for 4 hr day⁻¹ 5 day wk⁻¹ for 2 wk caused an increase in liver enzyme activity in the serum, indicating liver damage (18).

Gavage rat 150, 450 or 1500 mg kg⁻¹ day⁻¹ for 60 days, and 250, 1000 or 2000 mg kg⁻¹ day⁻¹ for 10 days caused enlarged liver and kidneys (19).

Teratogenicity and reproductive effects

Inhalation rabbit, lowest toxic concentration 1000 mg m⁻³ 24 hr day⁻¹ on days 7-20 of gestation caused post-implantation mortality and abortion (20).

Oral mouse, lowest toxic dose 12 mg kg⁻¹ day⁻¹ on days 12-15 gestation caused craniofacial teratogenic effects (21).

Metabolism and toxicokinetics

In rats, exposed by inhalation to 210 ng m⁻³ (methyl-¹⁴C-*p*-xylene) for 1 hr, distribution of radioactivity immediately after termination of exposure was highest in the kidneys, followed by subcutaneous fat, ischiatic nerve, blood, liver and lungs (22).

Genotoxicity

Salmonella typhimurium TA100 without metabolic activation negative (23).

Escherichia coli WP2 *uvr* A with and without metabolic activation negative (24).

In vitro Chinese hamster ovary cells chromosomal aberrations and sister chromatid exchanges negative (metabolic activation unspecified) (25).

In vivo mouse bone marrow cells, induction of micronuclei negative (18).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (26).

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (27).

Other comments

NIOSH has designated xylene an ototoxin. It can cause hearing loss, ringing in the ears or total deafness and its toxicity can be exacerbated by combined exposure with noise (28).

WHO guideline value for total xylenes in drinking water 500 $\mu\text{g l}^{-1}$ (29).

Physical properties, uses, occurrence, analysis, carcinogenicity, mammalian toxicity, metabolism and genotoxicity of xylenes reviewed (30,31).

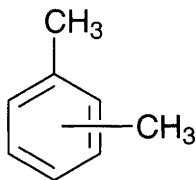
Environmental health criteria reviewed (32).

Autoignition temperature 530 °C.

References

1. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1991, **2**, 526-535.
2. Shell Chemie *Shell Industrie Chemicalien Gids* 1975, 's-Gravenhage, Netherlands.
3. Pickering, Q. H. et al *J. Water Pollut. Control Fed.* 1966, **38**(9), 1419.
4. Koenemann, W. H. *Quantitative Structure-Activity Relationships for Kinetics and Toxicity of Aquatic Pollutants and their Mixtures to Fish* 1979, Univ. Utrecht, Netherlands.
5. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
6. Vighi, M. et al *Chemosphere* 1987, **16**(5), 1043-1051.
7. Berville, P. E. et al in Verschuere, K. *Handbook of Environmental Data on Organic Chemicals* 2nd ed., 1983, 1191-1192, Van Nostrand Reinhold, New York, NY, USA.
8. Ogata, M. et al *Water Res.* 1978, **12**, 1041-1044.
9. Barker, J. F. et al *Groundwater Monit. Rev.* 1987 **7**, 64-72.
10. Ravischankara, A. R. et al *Int. J. Chem. Kinet.* 1978, **10**, 783-804.
11. Doyle, G. J. et al *Environ. Sci. Technol.* 1978 **9**, 237-241.
12. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behaviour of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
13. Abdul, A. S. et al *Hazard Waste Hazard Mat.* 1987, **4**, 211-221.
14. Vowles, P. D. et al *Chemosphere* 1987, **16**, 109-116.
15. Gekkon Yakuji 1980, **22**, 883.
16. *Biol. React. Intomed. Farmat. Tox. Inact. Proc. Int. Conf. Turku, Finland* 1977, 302.
17. Mohtashimpur, E. et al *Arch. Toxicol.* 1985, **58**, 106-109.
18. Patel, J. M. et al *Bull. Environ. Contam. Toxicol.* 1979, **21** 17-24.
19. Condie, L. W. et al *Drug Chem. Toxicol.* 1988, **11**(4), 329-354.
20. Ungary, G. et al *Arch. Toxicol.* 1985, **Suppl. 8**, 425.
21. *Abst. Papers Soc. Toxicol.* 1982, **19**, A22.
22. Carlsson, A. *Scand. J. Work Environ. Health* 1981, **7**, 51-55.
23. Klopman, G. et al *Mol. Toxicol.* 1987, **1**, 61-81.
24. Shimizu, H. et al *Jpn. J. Ind. Health* 1985, **27**, 400-419.
25. Rosenkranz, H. S. et al *Mutagenesis* 1990, **5**(6), 559-571.
26. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances Regulations* 1991, HMSO, London, UK.
27. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
28. *Chem. Health Saf.* 1997, **4**(2), 29.
29. *Guidelines for Drinking Water Quality* 2nd ed., 1993, **1**, WHO, Geneva, Switzerland.
30. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium.
31. IARC Monograph 1989, **47**, 125-156.
32. *Environmental Health Criteria No. 190: Xylenes* 1997, WHO/ICPS, Geneva, Switzerland

x8 xylene (mixed isomers)



C₈H₁₀

Mol. Wt. 106.17

CAS Registry No. 1330-20-7

Synonyms dimethylbenzene; methyltoluene; mixed xylenes; violet 3; xylol

EINECS No. 215-535-7

RTECS No. ZE 2100000

Uses Solvent. Gasoline blending. Organic synthesis.

Occurrence In fossil fuels. Identified in natural and drinking water (1,2).

Physical properties

B. Pt. 137-144°C **Flash point** 29°C **Specific gravity** 0.864 at 20°C with respect to water at 4°C

Partition coefficient log P_{ow} 3.1-3.2 **Volatility** v.p. 6.72 mmHg at 21°C ; v.den. 3.7

Solubility Water: almost insoluble. Organic solvents: acetone, benzene, diethyl ether, ethanol

Occupational exposure

DE-MAK 100 ppm (440 mg m⁻³)

FR-VME 100 ppm (435 mg m⁻³)

FR-VLE 150 ppm (650 mg m⁻³)

JP-OEL 100 ppm (430 mg m⁻³)

SE-LEVL 50 ppm (200 mg m⁻³)

SE-STEL 100 ppm (450 mg m⁻³)

UK-LTEL 100 ppm (441 mg m⁻³)

UK-STEL 150 ppm (662 mg m⁻³)

US-TWA 100 ppm (434 mg m⁻³)

US-STEL 150 ppm (651 mg m⁻³)

UN No. 1307 **HAZCHEM Code** 3M (flash point ≥23°C, ≤61°C, initial boiling point >35°C)

HAZCHEM Code 3ME (flash point <23°C, initial boiling point >35°C) **Conveyance classification** flammable liquid

Supply classification harmful

Risk phrases Flammable – Harmful by inhalation and in contact with skin – Irritating to the skin (R10, R20/21, R38)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with the eyes (S2, S25)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fathead minnow 16 mg l⁻¹, flow-through bioassay (3).

LC₅₀ (48 hr) golden orfe 110 mg l⁻¹, static bioassay (4).

Invertebrate toxicity

EC₅₀ (24 hr) *Photobacterium phosphoreum* Microtox test 79.4 µM (5).

LC₅₀ (24 hr) *Artemia salina* Artoxkit M test 1.82 mM (5).

LC₅₀ (24 hr) *Streptocephalus proboscideus* Streptoxkit F test 776 µM (5).

LC₅₀ (24 hr) *Brachionus calyciflorus* Rotoxkit F test 2.51 mM (5).

LC₅₀ (24 hr) *Daphnia magna* test 676 µM (5).

LC₅₀ (24 hr) freshwater snails *Amphimelania holandri* and *Lymnaea stagnalis* and freshwater crustaceans *Asellus aquiticus* and *Grammarus fossarum* 0.2070, 0.1720, 0.0270, and 0.0184 v/v, respectively (6).

Environmental fate

Nitrification inhibition

EC₅₀ (25 day) *Nitrosomonas* sp. 100 mg l⁻¹ (3).

Carbonaceous inhibition

LC₅₀ (5 day) aerobic heterotrophs isolated from activated sludge 1000 mg l⁻¹ (3).

Anaerobic effects

LC₅₀ (50 day) methanogenic bacterial cultures 250 mg l⁻¹ (3).

Degradation studies

Five Gram-negative bacterial strains able to degrade xylene were isolated from the industrial effluents of the ICI Plant and Nala Dek near Sheikhpura. NJ-3b2 and NJ-3c had common characters with Bacillaceae, NJ-3a with Enterobacteriaceae, and NJ-2f and NJ-3b1 could be affiliated to Vibrionaceae. Only NJ-3a, NJ-3b1, and NJ-3c harbour plasmids (7).

Degraded in standard biodegradability tests using sewage, activated sludge and seawater inocula (2).

Completely degraded in 8 days in groundwater in a gas-oil mixture. The acclimation period was 3-4 days (8).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 3600-5800 mg kg⁻¹ (9,10).

LC₅₀ (4 hr) inhalation rat 5000-6700 ppm (11,12).

LD₅₀ dermal rabbit ~4500 mg kg⁻¹ (13).

LD₅₀ intraperitoneal rat 1360-2500 mg kg⁻¹ (14,15).

LD_{Lo} oral human 50 mg kg⁻¹ (16).

Sub-acute and sub-chronic data

Oral rats, mice (14 day) 0, 125, 250, 500, 1000 or 2000 mg kg⁻¹ (rats); 0, 250, 500, 1000, 2000 or 4000 mg kg⁻¹ (mice).

Mortality occurred in high-dose rats and mice. High-dose rats and mice exhibited shallow breathing and prostration within 48 hr (17).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans or animals, IARC classification group 3 (1).

Gavage rats, mice (105 wk) 0, 250, 500 or 1000 mg kg⁻¹ (60% *m*-, 13% *p*-, 9% *o*-xylene, and 17% ethylbenzene, with 2.8 ppm benzene as impurity) 5 days wk⁻¹ for 103 wk. There was no significant difference in survival and tumour incidence between treated rats and mice and controls (17).

Gavage rats (141 wk) 0 or 500 mg kg⁻¹ (>99% purity, composition unspecified) 4 or 5 days wk⁻¹ for 104 wk.

Lymphomas were reported in 1/34 treated ♂ and 0/36 treated ♀, compared with 0/94 in controls. Other haemolymphoreticular tumours were reported in 4/34 treated ♂ and 3/36 ♀, compared with 3/45 and 1/49 in controls. The total number of animals with malignant tumours (type unspecified) at 141 wk was 14/38 treated ♂, 22/40 treated ♀, compared with 11/45 and 10/49 controls (18).

Teratogenicity and reproductive effects

Inhalation rat, lowest toxic dose 50 mg m⁻³ or 500 mg m⁻³ 6 hr day⁻¹ on days 1-21 of gestation resulted in embryotoxic and teratogenic disturbances. The brain, liver, lung and heart were affected. Post-implantation mortality was increased by 94% and 168% in the 50 and 500 mg groups, respectively, and the incidence of foetal skeletal abnormalities was increased by 62% and 177%, respectively. Gavage mice lowest toxic dose 21 mg kg⁻¹ day⁻¹ on days 6-15 of gestation increased the number of resorptions and malformations (cleft palate, wavy ribs) in treated animals (19).

Rat embryos explanted on day 9.5 of gestation and cultured in heat-inactivated rat serum to which xylene (0.1, 0.5 or 1.0 µl ml⁻¹) had been added showed no increase in malformations over controls, but there was clear evidence of embryotoxicity (20).

Using *in vitro* culture of postimplantation rat embryos (exposed to solvent for 40 hr of the organogenic period), xylene had a concentration-dependent embryotoxic effect at concentrations ≥ 1.89 mM (21).

Xylene vapour inhaled twice a day for 7 days in ♂ rats caused a decrease in the weight of the testes and accessory

reproductive organs, a decrease in acid phosphatase activity in the prostate and decreased plasma testosterone levels, compared with controls (22).

Metabolism and toxicokinetics

Xylenes are metabolised in the liver and lungs, primarily at the side chain, to form methylhippuric acid, methylbenzoic acid and glucuronides as the major metabolites. Methylbenzyl mercapturic acid was a minor metabolite. Xylenes are metabolised to a lesser extent at the aromatic ring to form dimethylphenol (23-27). When 250 mg of each isomer was administered intraperitoneally to rats, urinary excretion of thio-compounds was highest with *o*-xylene (27).

Following oral administration of 1.8 g of each of the 3 isomers to rabbits, >50% was metabolised and excreted in the urine within 24 hr (28).

Transplacental transfer occurred in mice exposed on days 11, 14 or 17 of gestation (10-min inhalation) (dose unspecified) (29).

Non-volatile metabolites accumulated in the nasal mucosa and olfactory bulb of the brain. The toxicological significance of these findings is discussed (30).

Irritancy

Dermal rabbit (24 hr) 500 mg caused moderate irritation. 5 mg instilled into rabbit eye for 24 hr caused severe irritation (31).

Vapour exposure human, (15 min) 2000 mg m⁻³ caused upper respiratory tract and eye irritation (32).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (33). *Escherichia coli* WP2s (λ) microscreen assay with and without metabolic activation negative (34).

Drosophila melanogaster sex-linked recessive lethal assay positive (35).

In vitro mouse lymphoma L5178Y tk⁺/tk⁻ forward mutation assay negative (metabolic activation unspecified) (36).

In vitro Chinese hamster ovary cells, chromosomal aberrations and sister chromatid exchanges with and without metabolic activation negative (37).

In vitro Chinese hamster V79 cells, inhibition of intercellular communication negative (metabolic activation unspecified) (38).

In vivo rat bone marrow cells chromosomal aberrations negative (35).

Other effects

Other adverse effects (human)

Exposure to xylene has been associated with increased risks of haematopoietic malignancies in 2 case-control studies. However, the number of cases was limited and the reported exposure was to a variety of compounds (1). Paint workers occupationally exposed suffered adverse effects to the central and peripheral nervous systems (1). Five adult healthy white men were exposed for 7 consecutive hours per day over 3 consecutive days to 40 ppm xylene in a controlled exposure chamber. This exposure was repeated three times at intervals of 2 weeks. Three different cytogenetic endpoints were evaluated using peripheral blood lymphocytes: number of sister chromatid exchanges, cell cycle delay, and cell mortality. No significant effects were observed. Exposure of human blood lymphocytes *in vitro* to xylene (0-2mM, 72 hr) did not result in significant effects at lower concentrations. At higher concentrations, only cell mortality was affected. The results indicate that exposure to low levels (within admissible limits) of xylene for a short period does not pose any potential mutagenic threat to humans (39). Spontaneous abortion, miscarriage and malformations have been reported following occupational exposure to xylene in the first trimester (40-42).

Any other adverse effects

Intraperitoneal rabbit, guinea pig, 1000 mg kg⁻¹ resulted in an increase in serum ornithine carbamyl transferase activity and lipid accumulation in the liver, indicating liver damage (43).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (44).
The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (45).

Other comments

NIOSH has designated xylene an ototoxin. It can cause hearing loss, ringing in the ears or total deafness and its toxicity can be exacerbated by combined exposure with noise (46).

Commercial grades typically contain: ~20% *o*-xylene, 40% *m*-xylene and 20% *p*-xylene, with ~15% ethylbenzene and smaller amounts of toluene, trimethylbenzene, phenol, thiophene, pyridine and non-aromatic hydrocarbons (1).

Physical properties, uses, occurrence, analysis, carcinogenicity, mammalian toxicity, metabolism and genotoxicity reviewed (1,47-51).

Environmental health criteria reviewed (52).

Flammable Hazard Index and Toxic Injury Potential concepts presented (53).

WHO guideline value for drinking water 500 $\mu\text{g l}^{-1}$ (54).

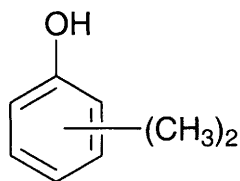
Autoignition temperature 490-550°C.

References

1. IARC Monograph 1989, **47**, 125-156.
2. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1991, **2**, 505-535, Lewis Publ., Chelsea, MI, USA.
3. Blum, D. J. W. et al *Res. J. Water Pollut. Control Fed.* 1991, **63**(3), 198-207.
4. di Vincenzo, G. D. et al *Am. Ind. Hyg. Assoc. J.* 1974, **35**, 21-29.
5. Calleja, M. C. et al *Food Chem. Toxicol.* 1994, **32**(2), 173-187.
6. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
7. Jabeen, N. et al *Sci. Int. (Lahore)* 1992, **4**(2), 189-193.
8. Knoepfeler, T. et al *Water Res.* 1978, **12**, 327-333.
9. *Gekkan Yakujii* 1980, **22**, 883.
10. Walf, M. A. et al *AMA Arch. Ind. Health* 1956, **14**, 387.
11. *Joint Assessments of Commodity Chemicals No. 6 Xylenes* 1986, European Chemical Industry Ecology and Toxicology Centre, Brussels, Belgium.
12. *Raw Mat. Data Hbk.* 1974, **1**, 123.
13. Carpenter, A. V. et al *Am. J. Ind. Med.* 1988, **13**, 351-362.
14. Hine, C. H. et al *Ind. Med.* 1970, **39**, 215-220.
15. Mohtashanipur, E. et al *Arch. Toxicol.* 1985, **58**, 106-109.
16. *Environ. Res.* 1986, **40**, 411.
17. *National Toxicology Program Research and Testing Division* 1997, Report No. TR-327, NIEHS, Research Triangle Park, NC, USA.
18. Montesano, R. et al (Eds.) *Long-term and Short-term Assays for Carcinogens: A Critical Appraisal* 1983, IARC, Lyon, France.
19. Marks, T. A. et al *J. Toxicol. Environ. Health* 1982, **9**, 97.
20. Brown-Woodman, P. D. C. et al *Ind. Health* 1991, **29**(4), 139-152.
21. Brown-Woodman, P. D. C. et al *Reprod. Toxicol.* 1994, **8**(2), 121-135.
22. Yamada, K. *Biol. Pharm. Bull.* 1993, **16**(4), 425-427.
23. Carlone, M. F. et al *Xenobiotica* 1974, **4**, 705-715.
24. Ogata, M. et al *Int. Arch. Occup. Environ. Health* 1980, **46**, 127-139.
25. Smith, B. R. et al *J. Pharmacol. Exp. Ther.* 1982, **223**, 736-742.
26. Tuftgarol, R. et al *Toxicologist* 1986, **39**, 225-345.
27. van Doorm, R. et al *Arch. Toxicol.* 1980, **43**, 293-304.
28. Bray, H. G. et al *J. Biochem.* 1949, **48**, 241-244.
29. Ghantous, H. et al *Biol. Res. Prog.* 1986, **7**, 98-105.
30. Dencker, L. et al *Pharmacol. Toxicol. (Copenhagen)* 1990, **66**(2), 87-92.
31. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
32. Carpenter, C. P. et al *Toxicol. Appl. Pharmacol.* 1975, **33**, 543-558.
33. Zeiger, E. et al *Environ. Mutagen.* 1987, **9**(Suppl. 9), 1-109.

34. Rossman, T. G. et al *Mutat Res.* 1991, **260**, 349-367.
35. Donner, M. et al *Mutat Res.* 1990, **74**, 171-172.
36. Lebowitz, H. et al *Environ. Mutagen.* 1979, **164**, 263.
37. Zeiger, E. et al *Environ. Mol. Mutagen.* 1990, **16**(Suppl. 18), 1-14.
38. Agowi, T. et al *Mutat. Res.* 1986, **164**, 263.
39. Richer, C. L. et al *Int. Arch. Occup. Environ. Health* 1993, **64**(8), 581-585.
40. Taskimen, H. et al *Br. J. Ind. Med.* 1986, **43**, 199-205, 432.
41. Axelsson, G. et al *Br. J. Ind. Med.* 1984, **41**, 305-312.
42. Holmberg, P. C. et al *Int. Arch. Occup. Environ. Health* 1982, **50**, 371-376.
43. Kamlet, M. J. et al *Environ. Sci. Technol.* 1987, **21**(2), 149-155.
44. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
45. 1967 *Directive on Classification, Packaging, and Labelling of Dangerous Substances* 67/548/EEC; 6th Amendment EEC Directive 79/831/EEC; 7th Amendment EEC Directive 91/32/EEC 1991, HMSO, London, UK.
46. *Chem. Health Saf.* 1997, **4**(2), 29.
47. *Chemical Safety Data Sheets* 1989, **1**, 332-335, The Royal Society of Chemistry, London, UK.
48. Snyder, R. (Ed.) *Ethel Browning's Toxicity and Metabolism of Industrial Solvents* 2nd ed., **1**, 64-79, Elsevier, Amsterdam, Netherlands.
49. Low, L. K. et al *Toxicol. Ind. Health* 1989, **5**(1), 85-105.
50. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium.
51. *Dangerous Prop. Ind. Mater. Rep.* 1986, **6**(6), 2-11.
52. *Environmental Health Criteria No. 190: Xylenes* 1997, WHO/IPCS, Geneva, Switzerland.
53. Hauser, R. L. et al *J. Forensic Sci.* 1994, **39**(5), 1237-1246.
54. *Guidelines for Drinking Water Quality* 2nd ed., 1993, **1**, WHO, Geneva, Switzerland

x9 xyleneol



C₈H₁₀O

Mol. Wt. 122.17

CAS Registry No. 1300-71-6

Synonyms dimethylphenol

EINECS No. 215-089-3

RTECS No. ZE 5425000

Uses Anti-knock fuel additive. Bactericide. Polymerisation catalyst. Organic synthesis. Solvent.

Occurrence Constituent of cresylic acid.

Physical properties

M. Pt. 20-76°C (range of the 6 isomers) **B. Pt.** 203-226°C (range of the 6 isomers)

Partition coefficient log P_{ow} 2.3 **Volatility** v.p. 0.014-0.18 mmHg at 25°C

Solubility Water: 4.6-5.9 g l⁻¹ at 25°C. Organic solvents: benzene, chloroform, diethyl ether, ethanol

Occupational exposure

UN No. 2261 **HAZCHEM Code** 2X **Conveyance classification** toxic substance

Supply classification toxic, dangerous for the environment

Risk phrases Toxic in contact with skin and if swallowed – Causes burns – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R24/25, R34, R51/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S26, S36/37/39, S45, S61)

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) carp 5-10 mg l⁻¹, static bioassay (1).

Invertebrate toxicity

LC₅₀ (24 hr) *Daphnia magna* 150 mg l⁻¹, static bioassay (2).

Bioaccumulation

Calculated bioconcentration factor 29-75 indicates that environmental accumulation would not be significant (3).

Environmental fate

Degradation studies

Oxidised to the corresponding catechol by *Pseudomonas putida* F1 and *Pseudomonas* strain JS6 (4).

BOD₅ 31% of ThOD (5).

Abiotic removal

Reacts with photochemically produced hydroxyl radicals in the atmosphere, estimated t_{1/2} 1.9-7.2 hr (6).

Night-time reaction with atmospheric nitrate radicals in urban areas is estimated to be 250 × faster than the reaction with hydroxyl radicals (7).

Adsorption and retention

Calculated K_{oc} 37-765 indicate that adsorption to soil and sediments would not be significant (3).

Mammalian & avian toxicity

Acute data

LD_{Lo} oral human 5000 mg kg⁻¹ (8).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (9).

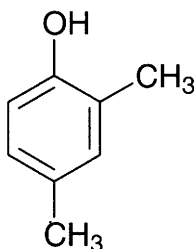
Other comments

Physical properties, uses, mammalian toxicity and safety precautions reviewed (10,11).

References

1. Bartle, K. D. et al *J. Chromatogr.* 1977, **135**, 351-358.
2. Grushko, Y. et al *Hydrobiological J.* 1975, **11**(5), 93-99.
3. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
4. Spain, J. C. et al *Appl. Environ. Microbiol.* 1988, **54**(6), 1399-1404.
5. CHRIS – Hazardous Chemical Data 1984-85, **2**, US Coast Guard, Dept. Transportation, Govt. Printing Office, Washington, DC, USA.
6. Atkinson, R. *Int. J. Chem. Kinet.* 1987, **19**, 799-828.
7. Carter, W. P. L. et al *Environ. Sci. Technol.* 1981, **15**, 829-831.
8. *Postgrad. Med. J.* 1986, **62**, 411.
9. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
10. *Chemical Safety Data Sheets* 1991, **4b**, 254-256.
11. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

X10 2,4-xyleneol



C₈H₁₀O

Mol. Wt. 122.17

CAS Registry No. 105-67-9

Synonyms 2,4-dimethylphenol; 4,6-dimethylphenol; 1-hydroxy-2,4-dimethylbenzene; *m*-xyleneol

EINECS No. 203-321-6

RTECS No. ZE 5600000

Uses Intermediate in manufacture of phenolic antioxidants. Pharmaceutical manufacturing. Plastics and resin manufacturing.

Physical properties

M. Pt. 22-23°C **B. Pt.** 211.5°C **Flash point** 96°C **Specific gravity** 1.036 at 20°C with respect to water at 4°C

Partition coefficient log *P*_{ow} 2.35

Solubility Water: 3.90 ppm. Organic solvents: ethanol

Occupational exposure

Supply classification toxic, dangerous for the environment

Risk phrases Toxic in contact with skin and if swallowed – Causes burns – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R24/25, R34, R51/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S26, S36/37/39, S45, S61)

Ecotoxicity

Fish toxicity

Median threshold limit (24 hr) crucian carp, tench, trout embryo 30, 13 and 28 mg l⁻¹, respectively (1).

LC₅₀ (96 hr) bluegill sunfish 7.8 mg l⁻¹ (2).

LC₅₀ (48 hr) fathead minnow 9.5 mg l⁻¹ (3).

LC₅₀ (24 hr) carp 30 mg l⁻¹ (4).

LC₅₀ (96 hr) tench 13 mg l⁻¹ (4).

Lethal aqueous exposure concentration rainbow trout 9.04 ± 0.32 mg l⁻¹; mean survival time 6.0 ± 1.7 h (5).

Invertebrate toxicity

EC₅₀ (2 day) *Tetrahymena pyriformis* 130.51 mg l⁻¹ (6).

LC₅₀ (48 hr) *Daphnia magna* 2.1 mg l⁻¹ (7).

LC₀ *Escherichia coli*, *Scenedesmus* sp. and *Daphnia* sp. 500, 40 and 24 mg l⁻¹, respectively (4).

EC₅₀ (5-30 min) *Photobacterium phosphoreum* 2.67 mg l⁻¹ Microtox test (8).

IC₅₀ (24 hr) *Daphnia magna* 11 mg l⁻¹ (9).

Bioaccumulation

The calculated bioconcentration factor of log 2.18 indicates that environmental accumulation is unlikely (10).

Environmental fate

Carbonaceous inhibition

Inhibition of glucose degradation by *Pseudomonas fluorescens* and *Escherichia coli* at 40 and 500 mg l⁻¹, respectively (11).

Degradation studies

Adapted activated sludge at 20°C, product is sole carbon source: 94.5% COD removal at 28.2 mg COD g⁻¹ dry inoculum hr⁻¹ (12).

20-200 mg l⁻¹ in prereduced medium using 10% v/v inoculum of municipal digester sludge underwent no significant mineralisation of added substrate and inhibited methanogenesis (13).

Readily biodegraded by soil bacteria indigenous to a spill site (14).

Degrades by hydroxylation at the 2- and 4-position to give protocatechuate, which is metabolised by fission of the benzene nucleus (15).

EC₅₀ activated sludge, modified OECD Method 209 respiration inhibition test, 190 mg l⁻¹ less than solubility, therefore unlikely to inhibit microorganisms in activated sludge process when present at concentrations in domestic wastewaters, provided that it does not behave as a competitive inhibitor (16).

Biodegradable (17).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 809, 3200 mg kg⁻¹, respectively (18).

LD₅₀ dermal mouse, rat 1040 mg kg⁻¹ (18,19).

LD₅₀ intravenous mouse 100 mg kg⁻¹ (20).

LD₅₀ intraperitoneal mouse 183 mg kg⁻¹ (21).

Carcinogenicity and chronic effects

Dermal ♀ mice 25 µl twice wkly following initiation by 0.3% 9,10-dimethyl-1,2-benzanthracene in benzene. Of the 28/30 survivors, 50% had papillomas (average 1.21 individual⁻¹) and 18% had malignant tumours at 23 wk (22).

Other comments

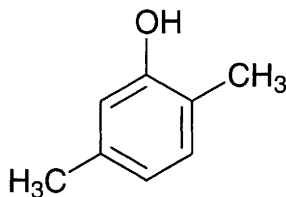
Reviews on human health effects, experimental toxicology and workplace experience listed (23).

References

1. Dore, M. et al *La Tribune du Cebedeau* 1975, **28**(374), 3-11.
2. Buccafusco, R. J. et al *Bull. Environ. Contam. Toxicol.* 1981, **26**, 446.
3. Phipps, J. L. et al *Bull. Environ. Contam. Toxicol.* 1981, **26**, 585.
4. Meinck, F. et al *Les Eaux Residuaire Industrielle* 1970.
5. Bradbury, S. P. et al *Environ. Toxicol. Chem.* 1989, **8**, 247-261.
6. Schultz, T. W. *Ecotoxicol. Environ. Saf.* 1987, **13**, 76.
7. LeBlanc, G. A. *Bull. Environ. Contam. Toxicol.* 1980, **24**, 684-691.
8. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
9. Devillers, J. *Sci. Total. Environ.* 1988, **76**, 79-83.
10. Isnard, P. et al *Chemosphere* 1988, **17**(1), 21-34.
11. Bringmann, G. et al *GWF, Gas- Wasserfach: Wasser/Abwasser* 1960, **81**, 337.
12. Pitter, P. *Water Res.* 1976, **10**, 231-235.
13. O'Connor, O. A. et al *Environ. Toxicol. Chem.* 1989, **8**(10), 853-862.
14. Mueller, J. G. et al *Appl. Environ. Microbiol.* 1991, **57**(5), 1277-1285.
15. Chapman, P. J. et al *Biochem. J.* 1968, **110**, 491-498.
16. Volskay, V. T. J. *Water Pollut. Control. Fed.* 1988, **60**(10), 1850-1856.
17. *Ministry of International Trade and Industry (MITI)* 1984, Japan.
18. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals Under Single Exposure* 1982, CIP, Moscow, USSR.
19. *Gig. Tr. Prof. Zabol.* 1974, **18**(2), 58.
20. *J. Med. Chem.* 1980, **23**, 1350.
21. *J. Med. Chem.* 1975, **18**, 868.

22. Baitwell, R. K. et al *Cancer Res.* 1959, 19, 413-424.
23. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

x11 2,5-xyleneol



C₈H₁₀O

Mol. Wt. 122.17

CAS Registry No. 95-87-4

Synonyms 6-methyl-*m*-cresol; 2,5-dimethylphenol; 3,6-dimethylphenol; 2,5-DMP; *p*-xyleneol; 1,2,5-xyleneol

EINECS No. 202-461-5

RTECS No. ZE 5775000

Uses Antiknock fuel additive.

Occurrence In coal tar.

Physical properties

M. Pt. 75-77°C **B. Pt.** 212°C **Specific gravity** 0.965 at 80°C **Partition coefficient** log *P*_{ow} 2.34

Volatility v.p. 10 mmHg at 91.3°C

Solubility Water: 3.2 g l⁻¹ at 25°C. Organic solvents: benzene, diethyl ether, ethanol

Occupational exposure

UN No. 2261 **HAZCHEM Code** 2X **Conveyance classification** toxic substance

Supply classification toxic, dangerous for the environment

Risk phrases Toxic in contact with skin and if swallowed – Causes burns – Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R24/25, R34, R51/53)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – Avoid release to the environment. Refer to special instructions/safety data sheet (S1/2, S26, S36/37/39, S45, S61)

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) carp 30 mg l⁻¹ (1).

LC₅₀ (96 hr) rainbow trout 3.2-5.6 mg l⁻¹ (2).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 9.1 ppm Microtox test (3).

IC₅₀ (24 hr) *Daphnia magna* 9.2 mg l⁻¹ (4).

Bioaccumulation

Calculated bioconcentration factor of 35 indicates that environmental accumulation is unlikely (5).

Environmental fate

Degradation studies

Removal from contaminated groundwater effected by treatment in upflow aerated columns and rotating disc biological contactors. Mechanisms involved were biodegradation at moderate levels. Volatilisation and adsorption were significant at higher levels (6).

BOD₁₀ 11.2% of ThOD (7).

Metabolised by *Pseudomonas* sp. yielding 3-hydroxy-4-methylbenzoic acid (8).

Abiotic removal

Reacts with photochemically produced hydroxyl radicals in the atmosphere, estimated $t_{1/2}$ 3.6 hr (9).

Adsorption and retention

Calculated K_{oc} 41 and 450 indicate low adsorption to soil and sediments (5).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat, rabbit 380, 440, 940 mg kg⁻¹, respectively (10).

Carcinogenicity and chronic effects

Dermal mouse, induced epithelial cell carcinoma when applied with 3,4-benzopyrene over 100 days. When applied alone, 3,4-benzopyrene did not induce pathological lesions (details not given) (11).

Metabolism and toxicokinetics

May be absorbed by ingestion, inhalation or via the skin (species unspecified) (12).

Metabolites identified in rabbits were 2,5-dimethylphenyl sulfate and 2,5-dimethyl- β -D-glucuronide (13).

Genotoxicity

Salmonella typhimurium TA98, TA100 with and without metabolic activation negative (14).

Other effects

Other adverse effects (human)

Extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and oedema of the larynx and bronchi (12).

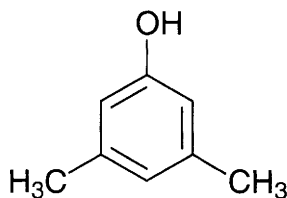
Other comments

Environmental and mammalian toxicity reviewed (1).

References

1. *Dangerous Prop. Ind. Mater. Rep.* 1984 **4**(1), 102-106.
2. Webb, M. et al *Water Res.* 1976, **10**, 303-306.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(4), 361-431.
4. Devillers, J. et al *Chemosphere* 1987, **16**(6), 1149-1163.
5. Lyman, W. K. et al *Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds* 1982, McGraw-Hill, New York, NY, USA.
6. van der Hoek, J. P. et al *Environ. Technol. Lett.* 1989, **10**(2), 185-194.
7. Singer, P. C. et al *Treatability and Assessment of Coal Conversion Wastewaters: Phase 1* 1979, US EPA-600/7-79-248.
8. Hopper, D. J. et al *Biochem. J.* 1971, **122**, 19.
9. Atkinson, R. *Int. J. Chem. Kinet.* 1987, **19**, 799-828.
10. *Hyg. Sanit.* 1968, **33**(9), 329.
11. Kaiser, H. E. *Cancer (Philadelphia)* 1967, **20**(5), 614-616.
12. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **1**, 1403, Sigma-Aldrich, Milwaukee, WI, USA.
13. Bray, H. G. et al *Biochem. J.* 1950, **47**, 395.
14. Epler, J. L. et al *Environ. Health Perspect.* 1979, **30**, 179-184.

X12 3,5-xylenol



$C_8H_{10}O$

Mol. Wt. 122.17

CAS Registry No. 108-68-9

Synonyms 3,5-dimethylphenol; 3,5-DMP; 1,3,5-xylenol; *sym-m*-xylenol

EINECS No. 203-606-5

RTECS No. ZE 6475000

Uses Solvent.

Occurrence In coal tars.

Physical properties

M. Pt. 65-66°C **B. Pt.** 222°C **Specific gravity** 0.9680 at 20°C with respect to water at 4°C

Partition coefficient $\log P_{ow}$ 2.35 **Volatility** v.p. 1 mmHg at 62°C

Solubility Water: 4.8 g l⁻¹. Organic solvents: benzene, chloroform, diethyl ether, ethanol

Occupational exposure

UN No. 2261 **HAZCHEM Code** 2X **Conveyance classification** toxic substance

Supply classification toxic

Risk phrases Toxic in contact with skin and if swallowed – Causes burns (R24/25, R34)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – In case of contact with eyes, rinse immediately with plenty of water and seek medical advice – After contact with skin, wash immediately with plenty of water – Wear suitable protective clothing, gloves and eye/face protection – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S26, S28, S36/37/39, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (24 hr) goldfish, crucian carp, tench 34-53 mg l⁻¹ (1,2).

Invertebrate toxicity

EC₅₀ (30 min) *Photobacterium phosphoreum* 12.5 ppm Microtox test (3).

IC₅₀ (24 hr) *Daphnia magna* 17.5 mg l⁻¹ (4).

Environmental fate

Degradation studies

Aerobic degradation was studied in a biofilm reactor to establish kinetic constants under conditions where 3,5-xylenol was the sole carbon source. At concentrations of ≤ 50 $\mu\text{g l}^{-1}$ reactions are governed by first-order reaction kinetics. Degradation of concentrations > 200 $\mu\text{g l}^{-1}$ are governed by zero-order reaction kinetics (5). BOD₁₀ 5.4% ThOD; ThOD 2.619 (6,7).

Metabolised by *Pseudomonas* sp. yielding 3-hydroxy-5-methylbenzoic acid (8).

Abiotic removal

Reacts with photochemically produced hydroxyl radicals in the atmosphere, estimated $t_{1/2}$ ~2 hr (9).

Adsorption and retention

Measured K_{oc} values 190-1400 in various soils (10,11).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird >110 mg kg (12).

LD₅₀ oral mouse, rat, rabbit 480, 600, 1300 mg kg⁻¹, respectively (13,14).

LD₅₀ intraperitoneal mouse 160 mg kg⁻¹ (15).

Carcinogenicity and chronic effects

Dermal mouse (100 day) when applied with 3,4-benzopyrene induced epithelial cell carcinoma. 3,4-benzopyrene did not induce any pathological lesions when applied alone (details not given) (16).

Metabolism and toxicokinetics

May be absorbed by ingestion, inhalation or via the skin (species unspecified) (17).

Metabolites identified in the rabbit were: 3,5-dimethylphenyl- β - β -glucuronide, 3,5-dimethylphenyl sulfate and 2,6-dimethylquinal (18).

Irritancy

725 μ g instilled into rabbit eye caused severe irritation (exposure unspecified) (19).

Other effects

Other adverse effects (human)

Extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema (17).

Legislation

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (20).

Other comments

Environmental and mammalian toxicity reviewed (21).

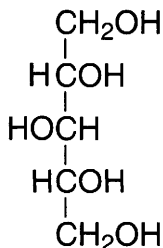
Reviews on human health effects, experimental toxicology, physico-chemical properties listed (22).

References

1. Lipnick, R. L. et al *Xenobiotica* 1987, **17**(8), 1011-1025.
2. *Water Res.* 1973, **7**, 929-941.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. Devillers, J. et al *Chemosphere* 1987, **16**(6), 1149-1163.
5. Arvin, E. et al *Water Sci. Technol.* 1991, **23**(7-9), 1375-1384.
6. Singer, P. C. et al *Treatability and Assessment of Coal Conversion Wastewaters: Phase I* 1979, USEPA-600/7-79-248.
7. Meinck, F. et al *Les Eaux Residuares Industrielles* 1970.
8. Hopper, D. J. et al *Biochem. J.* 1971, **122**, 19.
9. Atkinson, R. *Int. J. Chem. Kinet.* 1988, **19**, 799-828.
10. Goerlitz, D. F. et al *Environ. Sci. Technol.* 1985, **19**, 955-961.
11. Southworth, G. R. et al *Water, Air, Soil, Pollut.* 1986, **28**, 239-248.
12. Schafer, E. W. et al *Arch. Environ. Contam. Toxicol.* 1983, **12**, 355-382.
13. *Hyg. Sanit.* 1968, **33**(9), 329.
14. *Gig. Tr. Prof. Zabol.* 1972, **8**, 145.
15. *J. Med. Chem.* 1975, **18**, 868.
16. Kaiser, H. E. *Cancer (Philadelphia)* 1967, **20**(5), 614-616.
17. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **1**, 1404, Sigma-Aldrich, Milwaukee, WI, USA.
18. Bray, H. G. et al *Biochem. J.* 1950, **47**, 395.
19. *Am. J. Ophthalmol.* 1946, **29**, 1363.

20. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations 1991*, HMSO, London, UK.
21. *Dangerous Prop. Ind. Mater. Rep.* 1984, 4(1), 102-106.
22. ECETOC Technical Report No. 71 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

x13 xylitol



$\text{C}_5\text{H}_{12}\text{O}_5$

Mol. Wt. 152.15

CAS Registry No. 87-99-0

Synonyms xylit; *meso*-xylitol

EINECS No. 201-788-0

RTECS No. ZF 0800000

Uses Sweetener in confectionery and oral pharmaceuticals. In anticaries preparations.

Occurrence Microbial metabolite of xylose. Intermediate in the metabolism of glucose through the glucuronate cycle in the liver.

Physical properties

M. Pt. 95-97°C

Solubility Water: very soluble. Organic solvents: ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 13, 22 g kg⁻¹, respectively (1-3).

LD₅₀ intraperitoneal mouse 22 g kg⁻¹ (4).

LD₅₀ intravenous mouse, rabbit 3800, 4000 mg kg⁻¹, respectively (4,5).

Metabolism and toxicokinetics

May be absorbed by ingestion, inhalation or via the skin (6).

Genotoxicity

Salmonella typhimurium Ames test negative (details not given) (7).

Other effects

Other adverse effects (human)

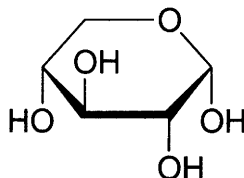
Large oral doses may cause diarrhoea and flatulence. Intravenous infusion may lead to hyperoxaluria, hyperuricaemia, changes in liver function tests and acidosis (8).

References

1. Salminen, S. et al *Toxicol. Lett* 1983, 18(Suppl. 1), 37.
2. *Drugs in Japan. Ethical Drugs* 1990, 294, Jakuggo Jiho Co. Tokyo, Japan.

3. *Gig. Sanit.* 1971, **36**(2), 25.
4. *Russ. Pharmacol. Toxicol.* 1971, **34**, 124.
5. *Fed. Prod. Fed. Am. Soc. Exp. Biol.* 1972, **31**, 726.
6. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3622, Sigma-Aldrich, Milwaukee, WI, USA.
7. Bakale, G. et al *Carcinogenesis* 1987, **8**(2), 253-264.
8. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK

X14 D-xylose



C₅H₁₀O₅

Mol. Wt. 150.13

CAS Registry No. 58-86-6

Synonyms wood sugar; xylomed; Xylo-Pfan; (+)-xylose

EINECS No. 200-400-7

RTECS No. ZF 2285000

Uses Sweetener. In tanning. Production of xylitol and ethanol by fermentation. Inhibitor in pharmaceuticals. Diagnostic agent used to investigate malabsorption from the gastro-intestinal tract.

Occurrence Widely distributed among plant materials, particularly in wood, straw and hulls in the form of the polysaccharide xylan. A constituent of glycosides.

Physical properties

M. Pt. 156-158°C **Specific gravity** 1.525 at 20°C with respect to water at 4°C

Solubility Water: 125% w/w. Organic solvents: ethanol, pyridine

Environmental fate

Degradation studies

Anaerobic degradation to methane in a mesophilic regime examined (1).

Although it is generally accepted that *Saccharomyces cerevisiae* cannot assimilate D-xylose, 4 strains utilised xylose aerobically (≤69% over 7 days) when co-metabolised with other substrates (2).

Metabolised by *Candida* sp. under fully aerobic and semi-aerobic conditions. Ethanol was produced only under semi-aerobic conditions (3).

Degraded more rapidly than L-xylose by oral bacteria (4).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 23 g kg⁻¹ (5).

LD₅₀ intravenous mouse 11 g kg⁻¹ (5).

Metabolism and toxicokinetics

Incompletely absorbed from the gastro-intestinal tract in humans. Absorbed xylose is partly metabolised mainly to carbon dioxide and water (6).

Following oral administration of 5 g to human adults, ≥26% of the dose was detected in the urine 5 hr after administration (7).

Other effects

Other adverse effects (human)

Large doses may cause gastro-intestinal discomfort. Administration of other drugs may effect absorption, interfering with the xylose test (6).

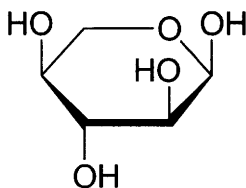
Any other adverse effects

Administration to rats has led to xylose entering the aqueous humour from the general circulation. Cataracts have been reported (8).

References

1. Sklyon, V. I. et al *Biotehnologiya* 1987, **3**(1), 79-85 (Russ.) (*Chem. Abstr.* **106**, 212515d).
2. Van Zyl, C. et al *J. Gen. Microbiol.* 1989, **135**(11), 2791-2798.
3. Alexander, M. A. et al *Appl. Microbiol. Biotechnol.* 1988, **28**(4-5), 478-486.
4. Izumori, K. et al *Kagawa Daigaku Nogakuba Gakavaiitsu Hokoku* 1987, **39**(1), 83-86 (Japan.) (*Chem. Abstr.* **111**, 170854j).
5. *Yakkyoku* 1981, **32**, 1367.
6. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
7. Iglesias, E. R. et al *Rev. Soc. Esp. Quim. Clin.* 1991, **10**(1), 27-29 (Span.) (*Chem. Abstr.* **115**, 274981x).
8. Grant, W. M. *Toxicology of the Eye* 2nd ed., 1974, 1090, Charles C. Thomas, Springfield, IL, USA

X15 L-xylose



$C_5H_{10}O_5$

Mol. Wt. 150.13

CAS Registry No. 609-06-3

EINECS No. 210-174-1

Occurrence Metabolite of L-ascorbic acid.

Physical properties

M. Pt. 150-152°C

Environmental fate

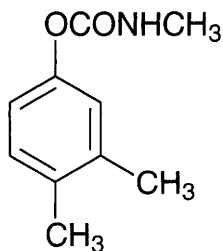
Degradation studies

Microbial degradation in soils proceeds at a slower rate than that of natural carbohydrates (1).

References

1. Izumori, K. et al *Kagawa Daigaku Nogakuba Gakavaiitsu Hokoku* 1987, **39**(1), 83-86 (Japan.) (*Chem. Abstr.* **111**, 170854j)

X16 xylylcarb



C₁₀H₁₃NO₂

Mol. Wt. 179.22

CAS Registry No. 2425-10-7

Synonyms Meobal; MPCM; S-1046; 3,4-xylyl methylcarbamate; 3,4-dimethylphenyl methylcarbamate; V17004

EINECS No. 219-364-9

RTECS No. FC 8750000

Uses Insecticide.

Physical properties

M. Pt. 79-80°C **Volatility** v.p. 5.3×10^{-4} mmHg at 20°C

Solubility Water: 580 mg l⁻¹ at 20°C. Organic solvents: acetone, acetonitrile, chloroform, cyclohexanone, ethanol, kerosene, toluene, xylene

Occupational exposure

Supply classification harmful

Risk phrases Harmful if swallowed (R22)

Safety phrases Keep out of reach of children (if sold to general public) (S2)

Ecotoxicity

Fish toxicity

LC₅₀ (48 hr) carp 10 mg l⁻¹ (1).

Environmental fate

Abiotic removal

Undergoes hydrolysis in alkaline media (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 60, 325-375 mg kg⁻¹, respectively (1,3).

LD₅₀ dermal rat, mouse >1000 mg kg⁻¹ (1,4).

LD₅₀ subcutaneous mouse 110 mg kg⁻¹ (5).

Genotoxicity

Bacillus subtilis rec assay negative (6).

Other effects

Any other adverse effects

Cholinesterase inhibitor (2).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (7).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (8).
WHO Toxicity Class II (9).

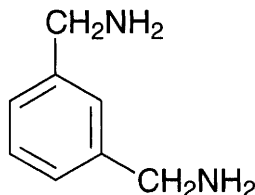
Other comments

Acute toxicity is potentiated by malathion (10).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
3. *Guide to Chemicals Used in Crop Protection* 1973, 6, 218.
4. *Sangyo Igaku* 1972, 19, 441.
5. *Toho Igakkai Zasshi* 1970, 17, 60.
6. *EPA Genotoxicity Program* 1988.
7. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
8. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
9. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
10. Takahashi, H. et al *Fundam. Appl. Toxicol.* 1987, 8(3), 415-442

x17 *m*-xylylenediamine



$\text{C}_8\text{H}_{12}\text{N}_2$

Mol. Wt. 136.20

CAS Registry No. 1477-55-0

Synonyms *m*-xylene- α,α' -diamine; 1,3-benzenedimethanamine; MXDA; *m*-phenylenebis(methylamine)

EINECS No. 216-032-5

RTECS No. PF 8970000

Uses Bactericide. Cross-linking agent.

Physical properties

M. Pt. 141°C **B. Pt.** 265°C at 745 mmHg **Flash point** 134°C (open cup) **Specific gravity** 1.032

Volatility v.p. 15 mmHg at 145°C

Solubility Water: miscible. Organic solvents: ethanol

Occupational exposure

FR-VLE 0.1 mg m^{-3}

US-TWA ceiling limit 0.1 mg m^{-3}

UN No. 3267

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 1600 mg kg⁻¹ (1).

LC₅₀ (1 hr) inhalation rat 700 ppm (2).

LD₅₀ dermal rabbit 2000 mg kg⁻¹ (2).

Inhalation rat (1 hr) 1740-6040 mg m⁻³ caused eye irritation, lachrymation and laboured breathing. Some deaths occurred 2-14 days after exposure. ♀ rats showed reduced weight gain. At necropsy lung, liver and kidney damage was observed (2).

Metabolism and toxicokinetics

May be absorbed by ingestion, inhalation and via the skin (species unspecified) (3).

Irritancy

Dermal rabbit (24 hr) 200 mg caused severe irritation. 50 µg instilled into rabbit eye for 24 hr caused severe irritation (1).

Other effects

Other adverse effects (human)

Extremely destructive to tissues of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema (3).

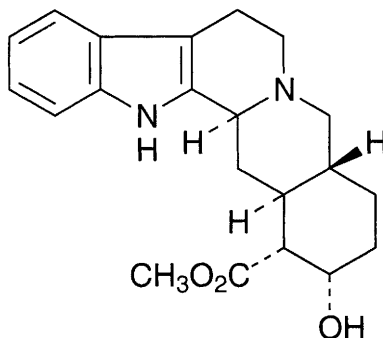
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (4).

References

1. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Propravku* 1972, Prague, Czechoslovakia.
2. *Documentation of Threshold Limit Values for Substances in Workroom Air* 4th ed. 1980, 440, American Conference of Governmental Industrial Hygienists, Cincinnati, OH, USA.
3. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, 2, 3623, Sigma-Aldrich, Milwaukee, WI, USA.
4. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

Y1 (+)-yohimbine



$C_{21}H_{26}N_2O_3$

Mol. Wt. 354.45

CAS Registry No. 146-48-5

Synonyms Aphrodine; Aphrosol; Coryrine; methyl 17-hydroxy-yohimban-16-carboxylate; Quebrachine; yohimbic acid methyl ester

EINECS No. 205-672-0

RTECS No. ZG 1000000

Uses Reversal of anaesthesia. Adrenergic blocking agent. Has been used as an aphrodisiac.

Occurrence Principal alkaloid of the bark of the yohimbe tree. Found in Rubiaceae and related trees, also in *Rauwolfia serpentina* (L.).

Physical properties

M. Pt. 231-233°C

Solubility Water: sparingly soluble. Organic solvents: benzene, chloroform, diethyl ether, ethanol

Ecotoxicity

Fish toxicity

Caused loss of equilibrium in stickleback in 16-24 hr at a concentration of 5 mg l⁻¹. Fatal to stickleback, brown trout and sockeye salmon in 3-4 hr at 10 mg l⁻¹. Test conditions: total hardness 0-17 mg l⁻¹; methyl orange alkalinity 14 mg l⁻¹; and pH 7.6 (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, cat 43, 51 mg kg⁻¹, respectively (2,3).

LD₅₀ subcutaneous cat 37 mg kg⁻¹ (3).

LD₅₀ intraperitoneal mouse, cat 16 mg kg⁻¹ (3).

Metabolism and toxicokinetics

Following intravenous administration to rats, yohimbine entered the brain very rapidly and disappeared from the brain with a t_{1/2} of 7.7 hr (4).

Other effects

Other adverse effects (human)

Yohimbine produces an α₂-adrenoceptor block of short duration. It produces an antidiuretic action, increases heart rate and blood pressure, and orthostatic hypotension. It has been reported to cause anxiety and manic reactions (5).

Any other adverse effects

Administration of 0, 2, 4 or 8 mg kg⁻¹ to rats (route unspecified) affected EEG frequency and power in the ♀, (α and β bands) (6).

Intracerebral ♂ rat, 5-100 µg animal⁻¹ or intraperitoneal ♂ rat 0.35-10 mg kg⁻¹ stimulated sexual behaviour. Maximum stimulating doses were 15 µg and 1.0 mg kg⁻¹, respectively. The results indicated the importance of central nervous system mechanisms (7).
 Injection of 5 mg kg⁻¹ to rats did not alter prepulse inhibition of the acoustic startle reflex (8).
 Intraperitoneal rat 0.5 or 1.5 mg kg⁻¹. The low dose enhanced learning of a food-motivated delayed-reinforcement autoshaping task, but it also increased conditioned behavioural arousal. The high dose retarded acquisition, but when it was withdrawn the animals learned; exploratory activity, however, was increased beyond control levels prior to acquisition (9).
 Tritiated yohimbine binds to α₂-adrenoceptors predominantly in the renal medulla in rats (10).

Other comments

It has been administered orally in the treatment of ♂ impotence for its alleged aphrodisiac properties, but convincing evidence of such an effect is lacking. It is contra-indicated in renal or hepatic disease (5).

References

1. McPhee, C. et al *Lethal Effects of 2014 Chemicals to Fish* 1989, EPA 560/6-89-001, PB 89-186-715, Washington, DC, USA.
2. *Pesticide Sci.* 1980, **11**, 555.
3. *Arzneim.-Forsch.* 1955, **5**, 432.
4. Hubbard, J. W. et al *Nauryn-Schmiedeberg's Arch. Pharmacol.* 1988, **337**(5), 583-587.
5. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
6. Enaiben, G. *Neuropsychobiology* 1990, **21**(4), 205-215.
7. Sala, M. et al *Physical. Behav.* 1990, **47**(1), 165-173.
8. Davis, M. et al *Psychopharmacology (Berlin)* 1988, **95**(2), 151-156.
9. Hueng, M. et al *Life Sci.* 1987, **41**(9), 1083-1088.
10. Takatori, K. et al *J. Int. Med. Res.* 1991, **18**(2), 153-160

Y2 yttrium

Y

Y **Mol. Wt.** 88.91 **CAS Registry No.** 7440-65-5
EINECS No. 231-174-8 **RTECS No.** ZG 2980000
Uses With other rare earths as phosphor for colour television receivers. Oxide for gas and acetylene lights.
Occurrence Occurrence in Earth's crust 29-36 ppm. Found principally as phosphate (xenotime), mixed oxides (fergusonite and samarskite) and silicates (yttrialite and gadolinite).

Physical properties

M. Pt. 1509°C **B. Pt.** 3200°C **Specific gravity** 4.472

Occupational exposure

FR-VME 1 mg m⁻³
UK-LTEL 1 mg m⁻³ **UK-STEL** 3 mg m⁻³
US-TWA 1 mg m⁻³

Mammalian & avian toxicity

Metabolism and toxicokinetics

In mice, yttrium has a high affinity for teeth and bones, where accumulation occurs and metabolism is slow (1).

Other comments

^{90}Y conjugated to monoclonal antibodies is being investigated for the treatment of ovarian cancer. It is suitable, as a colloidal suspension of the silicate, for instillation into pleural or peritoneal cavities in the treatment of malignant pleural effusion or malignant ascites (2).

Toxicity of rare-earth elements, including yttrium, reviewed (3).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (4).

References

1. Zhang, M. et al *Biol. Trace Chem. Res.* 1988, **17**, 81-90.
2. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
3. Filov, V. A. et al (Eds.) *Harmful Chemical Substances* 1993 **1**, 326-343, Ellis Horwood, New York, NY, USA.
4. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

Y3 yttrium chloride



Cl_3Y

Mol. Wt. 195.26

CAS Registry No. 10361-92-9

Synonyms yttrium trichloride

EINECS No. 233-801-0

RTECS No. ZG 3150000

Uses Catalyst. In superconductors.

Physical properties

M. Pt. 721°C B. Pt. 1507°C Specific gravity 2.180 (hexahydrate)

Solubility Water: miscible with water. Organic solvents: dimethyl sulfoxide, ethanol, pyridine

Occupational exposure

US-TWA 1 mg m⁻³ (as Y)

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat, guinea pig, mouse 45, 85, 90 mg kg⁻¹, respectively (1,2).

Metabolism and toxicokinetics

Following intratracheal administration to rats, pulmonary clearance $t_{1/2}$ for yttrium was 168 days (3).

Following i.v. administration to rats of 9-10 and 18-20 mg kg⁻¹, 78% of the dose was distributed into the liver, bone and spleen on day 1. High doses markedly increased accumulation in the spleen and lungs, and the calcium concentration in the liver, spleen and lungs. Yttrium chloride disappeared from the blood on day 1, but was retained in the organs. The percentage of the dose remaining in the liver was highest at 8 hr to 2 days, and then gradually decreased (4).

Irritancy

Irritating to the skin, eyes, mucous membranes and upper respiratory tract (species unspecified) (5).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA102, TA1537, TA2637 in combination with 9-aminoacridine negative (6).

Other effects

Other adverse effects (human)

Clinical manifestations of poisoning occurred in two stages. The first stage was characterised by dyspnoea and pulmonary oedema and the second by oedema of the liver, congestion of the portal vein, subpleural haemorrhages and hypoaemia of the lungs (7).

Legislation

Limited under EC Directive on drinking water quality 80/778/EEC. Chlorides: guide level 25 mg l⁻¹ (8).

UK maximum admissible concentration in drinking water, chloride 400 mg l⁻¹ (12-monthly average) (9).

References

1. *AMA Arch. Ind. Health* 1957, 16, 475.
2. *Arch. Environ. Health* 1962, 5, 437.
3. Kodama, N. et al *Toxicol. Appl. Pharmacol.* 1990, 104(2), 301-311.
4. Nakamura, Y. et al *Fundam. Appl. Toxicol.* 1997, 37(2), 106-116.
5. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, 2, 3626, Sigma-Aldrich, Milwaukee, WI, USA.
6. Iychara, O. H. et al *Jpn. J. Genet* 1987, 62(2), 159-162.
7. Filov, V. A. et al (Eds.) *Harmful Chemical Substances* 1993, 1 326-343, Ellis Horwood, New York, NY, USA.
8. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
9. SI 1989 No. 1147 *The Water Supply (Water Qualities) Regulations* 1989, HMSO, London, UK

Y4 yttrium nitrate



N₃O₉Y

Mol. Wt. 274.92

CAS Registry No. 10361-93-0

Synonyms yttrium trinitrate; yttrium (3+) nitrate; yttrium(III) nitrate

EINECS No. 233-802-6

RTECS No. ZG 3675000

Uses Catalyst. In superconductors.

Physical properties

Specific gravity 2.680 (tetrahydrate)

Solubility Water: soluble in water

Occupational exposure

US-TWA 1 mg m⁻³ (as Y)

UN No. 1477

UN No. 3218 (aqueous solution) **HAZCHEM Code 1** **HAZCHEM Code 2** (aqueous solution)

Conveyance classification oxidising substance

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat, mouse 350, 1700 mg kg⁻¹, respectively (1,2).

LD₅₀ intravenous rabbit 520 mg kg⁻¹ (2).

Sub-acute and sub-chronic data

Intraperitoneal rat 4-32 mg kg⁻¹ inhibited gastric secretia in a dose-dependent manner. Intragastric administration at the same dose rates caused serious gastric mucosal damage and decreased the secretion of alcian blue binding mucous in fasted rats (3).

Teratogenicity and reproductive effects

Intratesticular ♂ goat, lowest tissue dose, single injection of 5 mg kg⁻¹ reduced spermatogenesis (3).

Irritancy

Dermal rabbit (24 hr) 500 mg caused moderate irritation. 100 mg instilled into rabbit eye caused severe irritation (duration unspecified) (4).

Genotoxicity

In vivo goat sperm dominant lethal assay positive (3).

Other effects

Any other adverse effects

Intraperitoneal rat 4-32 mg kg⁻¹ inhibited gastric secretion in a dose-dependent manner. Intragastric administration at the same dose rates caused serious gastric mucosal damage and decreased the secretion of Alcian Blue binding mucous in fasted rats (5).

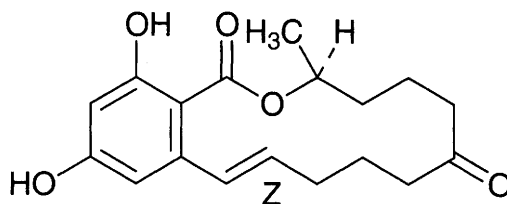
Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Nitrates: guide level 25 mg l⁻¹, maximum admissible concentration 50 mg l⁻¹ (6).

References

1. Cochran, et al *Arch. Ind. Hyg. Occup. Med.* 1950, 1, 637.
2. *Environ. Qual. Saf.* 1975, 1, 1.
3. *Indian J. Exp. Biol.* 1973, 11, 143.
4. *Acute Toxicity Data* 1993, 12, 629.
5. Luo, G. *Zhongguo Yadisa Yu Dulxue Zazhi* 1991, 5(1), 50-52 (Ch.) (*Chem. Abstr.* 115, 2727j).
6. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

Z1 zearalenone



$C_{18}H_{22}O_5$

Mol. Wt. 318.37

CAS Registry No. 17924-92-4

Synonyms compound F-2; 14,16-dihydroxy-3-methyl-7-oxo-*trans*-benzoxacyclotetradec-11-en-1-one; FES; (*E*)-3,4,5,6,9,10-hexahydro-14,16-dihydroxy-3-methyl-1*H*-2-benzoxacyclotetradecin-1,7(8*H*)-dione; fusarium toxin; 6-(10-hydroxy-6-oxo-*trans*-1-undecenyl)- β -resorcylic acid-*n*-lactone; mycotoxin F2; (-)-zearalenone; (*s*)-zearalenone; *trans*-zearalenone

EINECS No. 241-864-0

RTECS No. DM 2550000

Uses Veterinary anabolic. Chemical intermediate in the manufacture of zearalanol.

Occurrence Formed by *Fusarium* and *Giberella* species. Found in cereals and foodstuffs (1).

Physical properties

M. Pt. 161-162°C (L-form); 187-189°C (DL-form) **Partition coefficient** $\log P_{ow}$ 3.244 (2)

Solubility Water: 20 mg l⁻¹ at 25°C. Organic solvents: acetone, benzene, dichloromethane, diethyl ether, hexane, methanol

Ecotoxicity

Invertebrate toxicity

EC₅₀ (5-15 min) *Photobacterium phosphoreum* 13 ppm Microtox test (3).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, >16 g kg⁻¹ (4).

LD₅₀ intraperitoneal mouse 5 g kg⁻¹ (5).

Sub-acute and sub-chronic data

Rats were treated with 1, 3 or 5 mg kg⁻¹ day⁻¹ for 7 to 28 days. A dose- and time-dependent inhibition of body-weight gain was observed, although an anabolic effect was seen in rats given 1 mg kg⁻¹ day⁻¹ for 14 days (route unspecified) (6).

Oral, rat, mouse 30-3000 mg kg⁻¹ diet for 13 wk caused a dose-related increase in osteopetrosis (7).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, sufficient evidence for carcinogenicity to animals, IARC classification group 2A (8).

Oral rat, mouse (108 wk) 0, 50 or 100 mg kg⁻¹ diet for mice, 0, 25 or 50 mg kg⁻¹ diet for rats for 103 wk. A dose-related reduction in body-weight gain was observed in rats, but not in mice. Survival rates in treated animals were not significantly different from controls. No compound-related increase in tumour incidence was observed in treated rats. A small increase in hepatocellular adenomas was observed in mice, but this was statistically significant only in the high-dose ♀ mice. A statistically significant increase in pituitary adenomas occurred in ♂ and ♀ mice (7).

Teratogenicity and reproductive effects

There is evidence that the consumption of corn contaminated with zearalenone by turkeys and chickens can lead to vent enlargements and infertility (9).

Mice injected during the neonatal period suffered delayed vaginal opening, persistent anovulatory oestrus, and sterility. Infertility, accompanied by thickening of the vaginal epithelium, even after ovariectomy and adrenalectomy, indicating mucosal independence of endogenous oestrogens, resulted from daily dosing for 3-5 neonatal days. The hypothalamic-pituitary system appears to be affected as well as the sexual organs (10). ♂ and ♀ rat, 0.1, 1.0 or 10 mg kg⁻¹ diet. The high dose greatly impaired fertility of ♀ and increased foetal death and resorptions. No teratogenic response was observed (total exposure unspecified) (4).

Oral ♂ rat 1000 or 3000 mg kg⁻¹ diet for 13 wk caused atrophy of the seminal vesicles and testes, and fibromuscular hyperplasia of the prostate (7).

Gavage rat, 1, 5 or 10 mg kg⁻¹ day⁻¹ on days 6-15 of gestation. The high dose caused a significant reduction in foetal weight and an increase in minor skeletal anomalies in foetuses (11).

Oral guinea pig 7, 14 or 21 mg kg⁻¹ day⁻¹ on days 1-8 of gestation. The high dose caused foetal death. When administered at 20 or 30 mg kg⁻¹ day⁻¹ on days 1-3 or 4-5 or 6-8 of gestation, or 60 or 90 mg kg⁻¹ day⁻¹ on days 4-5 of gestation, all groups except those treated on days 1-3 had normal pregnancies (12).

Oral ♂ pig 2 or 10 µg kg⁻¹ diet for 7 wk did not affect libido, mating behaviour, plasma concentration of testosterone or spermatogenesis. A slight increase in secondary sperm abnormalities (mainly acrosome effects) was observed from wk 3-4. Thus, zearalenone at levels normally found in contaminated feed does not affect sexual behaviour and sperm quality of mature boars (13).

Feeds contaminated with zearalenone at a few mg total dose have caused a variety of reproductive disorders in swine, including vulvovaginitis, infertility and abortion (14).

Metabolism and toxicokinetics

Oral ♂ pig, 15 ppm diet for 2 wk. The metabolite zearalenol was detected in the liver, kidneys, urine and faeces together with unmetabolised zearalenone. The amount of α-zearalenol was always higher than the β-stereoisomer (15).

High protein diets in rats increased urinary excretion of zearalenone and its metabolites, thus ameliorating symptoms of toxicity (16).

The reduction of zearalenone to zearalenol is catalysed by a 3α-hydroxy-steroid dehydrogenase (17).

Irritancy

Dermal guinea pig (24 hr) 50 mg caused severe irritation (18).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537, TA1538 with and without metabolic activation marginally positive (19).

Escherichia coli K12 SOS Chromotest negative (20).

Saccharomyces cerevisiae genetic changes at *ade 2* locus, with or without metabolic activation negative (21).

In vitro mouse lymphoma L5178Y, tk⁺/tk⁻ forward mutation negative (22).

In vitro Chinese hamster ovary cells, without metabolic activation, sister chromatid exchanges and chromosomal aberrations positive; with metabolic activation negative (23).

Other effects

Other adverse effects (human)

The risk of oesophageal cancer correlates with corn contamination with the *Fusarium* mycotoxins zearalenone and deoxynivalenol. However, statistical evaluation of these data was not possible and the study was considered inadequate to evaluate the carcinogenicity of zearalenone to humans (1,24).

Any other adverse effects

Zearalenone and its metabolites bind to uterine cytoplasmic receptors and elicit the translocation of the cytosol-receptor complex into the nucleus (species unspecified). Zearalenone also binds to the mammary gland oestrogen receptor (7).

Zearalenone, a phytoestrogen, is 25-120× less potent than oestradiol in two *in vitro* test systems for oestrogenic activity (oestrogenic responsive cell proliferation and oestrogen-specific protein induction in MCF-7 cells) (14).

Oral administration suppressed the immune response to *Listeria monocytogenes* in mice (25).

Zearalenone is reported to promote cell proliferation and RNA and protein synthesis in the uterus of ovariectomised rats and mice (26,27).

Legislation

The log P_{ow} value exceeds the European Community recommended level 3.0 (6th and 7th amendments) (28).

Other comments

Environmental endocrine disruptor (29).

Physical properties, uses, occurrence, carcinogenicity, mammalian toxicity, metabolism and mutagenicity reviewed (1,30).

References

1. IARC Monograph 1983, **31**, 279-291.
2. McCoy, G. D. et al *Carcinogenesis* 1990, **11**(7), 111-1117.
3. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
4. Bailey, D. E. et al *Toxicol. Appl. Pharmacol.* 1976, **37**, 144.
5. *Vet. Hum. Toxicol.* 1983, **25**, 355.
6. Babic, L. et al *Veterinaria (Sarajevo)* 1989, **38**(3-4), 321-325 (Serbo-Croatian) (*Chem. Abstr.* **114**, 766979).
7. National Toxicology Program *Carcinogenic Bioassay of Zearalenone* 1982, NTP81-54, DHHS Publ. No. (NIH) 81-1791, Washington, DC, USA.
8. IARC Monograph 1987, **Suppl.7** 74.
9. Mirocha, C. J. et al in *Microbial Toxins* Kadis, S. et al (Eds.), Vol. 7, 1971, pp. 107-138, Academic Press, New York, NY, USA.
10. Ito, Y. et al *Cereal Res. Commun.* 1997, **25**(3, Pt.1), 453-454.
11. Ruddick, J. A. et al *Bull. Environ. Contam. Toxicol.* 1976, **15**, 678-681.
12. Long, G. G. et al *Am. J. Vet. Res.* 1989, **50**(8), 1220-1223.
13. Stolla, R. et al *Zuchthygiene* 1987, **22**(4), 165-172.
14. Mayr, U. et al *Toxicology* 1992, **74**, 135-149.
15. Lasztity, R. et al *Period. Polytech. Chem. Eng.* 1989, **33**(3-4), 203-209.
16. Fitzpatrick, D. W. et al *Nutr. Res. (N.Y.)* 1988, **8**(6), 663-671.
17. Olsen, M. et al *Acta Pharmacol. Toxicol.* 1981, **48**, 157-161.
18. *J. Assoc. Off. Analyst. Chem.* 1974, **57**, 1121.
19. Klopman, G. et al *Mutat. Res.* 1990, **220**, 1-50.
20. Auffray, Y. et al *Toxic. Assess.* 1988, **3**(4), 371-378.
21. Kuczuk, M. H. et al *Mutat. Res.* 1978, **53**, 11-20.
22. McGregor, D. B. et al *Environ. Mol. Mutagen.* 1988, **12**(1), 85-154.
23. Galloway, S. M. et al *Environ. Mol. Mutagen.* 1987, **10**(Suppl. 10), 1-175.
24. Marasas, W. F. D. et al *J. Agric. Food Chem.* 1979, **27**, 1108-1112.
25. Pestka, J. J. et al *Food Chem. Toxicol.* 1987, **25**(4), 297-304.
26. Cleno, Y. et al *Chem. Pharm. Bull.* 1974, **22**, 2830-2835.
27. Ueno, Y. et al *Jpn. J. Exp. Med.* 1975, **45**, 199-205.
28. 1967 Directive on Classification, Packaging, and Labelling of Dangerous Substances 67/548/EEC; 6th Amendment EC Directive 79/831/EEC; 7th Amendment EC Directive 91/32/EEC 1991, HMSO, London, UK.
29. IEH *Assessment on Environmental Oestrogens: Consequences to Human Health and Wildlife* 1995, Institute for Environment and Health, Leicester, UK.
30. Kuipeo-Goodman, T. et al *Regul. Toxicol. Pharmacol.* 1987, **7**(3), 253-306

Zn**Zn****Mol. Wt.** 65.39**CAS Registry No.** 7440-66-6**Synonyms** blue powder; enassay zinc dust; jasad; merrillite; rheinzink; pasco**EINECS No.** 231-175-3**RTECS No.** ZG 8600000**Uses** Plating for cathodic protection against corrosion of steel. In alloys. In galvanic cells and storage batteries. Reducing agent. Reagent in analytical chemistry.**Occurrence** Of 64 zinc minerals, the most important are sphalerite (zinc blende), zincite, smithsonite, wurtzite, calamine and goslarite. Abundance in Earth's crust: 0.02% by weight.

Occurs in a wide range of metalloenzymes.

Physical properties**M. Pt.** 419.5°C **B. Pt.** 908°C **Specific gravity** 7.140 at 25°C **Volatility** v.p. 1 mmHg at 487°C**Occupational exposure****UN No.** 1436 **HAZCHEM Code** 4Y **Conveyance classification** substance which in contact with water emits flammable gas, liable to spontaneous ignition**Supply classification** highly flammable (zinc dust pyrophoric)**Risk phrases** zinc dust – Flammable – Contact with water liberates extremely flammable gases – zinc dust pyrophoric – Contact with water liberates extremely flammable gases – Spontaneously flammable in air (R10, R15, R15, R17)**Safety phrases** Keep out of reach of children (if sold to general public) – Keep container tightly closed and dry – In case of fire, use class D fire extinguisher – never use water (S2, S7/8, S43)**Ecotoxicity****Fish toxicity**LC₅₀ (96 hr) brown trout <0.14 mg l⁻¹ in soft water at pH 8, 3.20 mg l⁻¹ in hard water at pH 5 (1).In preference-avoidance response determinations under uniform illumination in a countercurrent trough, lake Whitefish *Coregonus clupeaformis* avoided zinc ion concentrations > 10 µg l⁻¹ (2).**Invertebrate toxicity**LC₅₀ (48 hr) *Daphnia magna*, *Moina macrocopa*, *Paratya compressa improvisa* 0.12-1.6 mg l⁻¹ (3).

The growth of most soil microorganisms was significantly retarded at zinc levels of 0.1-0.2 ppm. Fungi were most resistant (4).

Primary production and cell multiplication were inhibited at 30 µg l⁻¹ in 2 green and 1 diatom freshwater algal species from Lake Ontario (5).EC₅₀ values for the reproduction of the springtail *Folsomia candida* Willem were determined after 6 wk exposure to zinc in an artificial soil. EC₅₀ (6 wk) 683 µg Zn g⁻¹ dry soil for total zinc in soil, corresponding to an internal concentration of 97 µg Zn g⁻¹ dry body weight. EC₅₀ (6 wk) 14 µg Zn g⁻¹ dry soil for water soluble zinc. The effects of a mixture of cadmium and zinc on growth were antagonistic, whilst the effects on reproduction were additive (6).**Bioaccumulation**The protectiveness of USEPA ambient water quality criteria for copper and zinc was tested using the snail *Leptoxis praerosa* in short and long-term artificial stream tests. Significant bioconcentration of both Cu and Zn occurred within 40 days and significant cellulolytic enzyme activity impairment within 54 days for both metals at the respective chronic criteria concentrations. Approximately additive effects were seen in combination treatment of Cu and Zn. Survival was much higher in the Cu-exposed snails. The authors concluded that the USEPA criteria

based upon abbreviated chronic tests may be underprotective for some sensitive taxa when exposures are prolonged (7).

Environmental fate

Nitrification inhibition

Inhibition of denitrification, threshold concentration 1 mg l⁻¹ rotating disc. Threshold for nitrification 10 mg l⁻¹ – rotating disc. Threshold for nitrification and denitrification in activated sludge 10 mg l⁻¹ (8,9).
25% Nitrification inhibition at 11 mg l⁻¹ in activated sludge (9).

Mammalian & avian toxicity

Acute data

Inhalation man (50 min) lowest toxic dose 124 mg m⁻³ – cough, dyspnea, increased sweating (10).

Carcinogenicity and chronic effects

Intratracheal instillation (2 yr) single dose of 25 or 50 mg (or repeated doses of 2 or 5 mg) induced sarcomas in the lungs and testicular tumours in 15% of treated animals (species unspecified) (4).

Metabolism and toxicokinetics

Factors which influence gastro-intestinal absorption include zinc status (absorption is increased during zinc deficiency), intracellular transport (the active transport mechanisms of zinc appears to be under metabolic control), ligands (zinc may be bound to several ligands, some of which impede and others enhance absorption) and endogenous zinc secretion (a significant amount of zinc is secreted into the intestinal lumen via the epithelial cells, bile and pancreatic secretion) (11).

Mean zinc concentrations in humans are: 1.1 mg l⁻¹ in blood plasma; 1.2 mg l⁻¹ in milk; 171 mg l⁻¹ in bile; 9.3-12 mg l⁻¹ in sweat; 6.4 mg l⁻¹ in urine; 690 mg l⁻¹ in seminal plasma; 0.03 mg l⁻¹ in cerebrospinal fluid; 40 µg g⁻¹ haemoglobin; 193 µg g⁻¹ hair (11).

Zinc does not appear to accumulate in the human body with age (12).

Gastro-intestinal absorption of zinc is inhibited by phytate, an organic phosphate compound present in grain and vegetable components of the human diet, with which zinc forms insoluble complexes at alkaline pH (13,14).

Zinc uptake by high molecular weight proteins in the intestinal mucosa is an active transport process requiring ATP (15).

Irritancy

Dermal human 300 µg day⁻¹ for 3 days caused mild irritation (16).

Genotoxicity

Salmonella typhimurium TA98, TA102, TA1535, TA1527 with and without metabolic activation negative (17).

In vivo mouse bone marrow and lymphocytes micronucleus assay positive (18).

Maize root meristem, 2-10-fold increase in zinc concentration decreased mitosis and increased chromosomal aberrations (19).

Other effects

Other adverse effects (human)

Zinc impaired the intestinal absorption of iron (20).

Several cases reported of excessive zinc intake having possible effects on the pancreas (11).

Excess zinc does not appear to cause liver or kidney damage (11).

Subjects administered 300 mg elemental zinc day⁻¹ for 6 wk (20 × above RDA) resulted in damage to the immune system. However, it is not clear whether damage was due to copper deficiency caused by the elevated zinc intake (11,21).

A combined study in France and Italy on the role of zinc and copper in breast cancer incidence, using hospital-based case controls as subjects, showed that blood zinc levels were consistently higher in cancer patients than in controls. Dietary intake of zinc was equivalent in all subjects (22).

A direct correlation between estimated zinc intake and age-adjusted mortality from leukaemia and cancers of the skin, breast, prostate and intestine. The study suggested that increased dietary zinc interfered with absorption and utilisation of dietary selenium, producing a relative selenium deficiency (23).

In contrast, in countries where wheat and corn are primary staples, low dietary levels of micronutrients, particularly zinc, magnesium and nicotinic acid correlate with a high risk of oesophageal cancer (24).

Any other adverse effects

Cats exposed by inhalation to zinc dust suffered pulmonary oedema and haemorrhage. Leucocytes and macrophages accumulated in the bronchioles and alveoli (4).

Total serum cholesterol was decreased in experimentally induced zinc deficiency in humans, while in rats ingestion of high levels of zinc increased serum cholesterol. This effect is believed to be due to copper deficiency which may be induced by excess zinc intake (25,26).

Clinical evidence indicates that neurological abnormalities do not typically occur in animals or humans exposed to higher than normal levels of zinc in air, water or food, although neurological effects and degenerative changes were observed when zinc wire was introduced into the ventricles of the brain of rats (11,27,28).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Zinc: guide level 100 µg l⁻¹ at supply works, 5000 µg l⁻¹ after 12 hr contact with consumers' pipework (29).

Included in Schedule 4 (Release into Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (30).

Zinc-derived coatings with zinc dust pigments, maximum lead content 100 ppm (Iowa Dept. Transport, USA) (31).

EEC Environmental Quality Objective (EQO) for fresh water used for direct abstraction to potable supply 3000 µg l⁻¹ total zinc (95% of samples). EQO for protection of sensitive aquatic life (e.g. salmonid fish) 8-125 µg l⁻¹ for soft and hard waters, respectively. EQO for protection for other aquatic life (e.g. cyprinid fish) 25-500 µg l⁻¹ for soft and hard waters, respectively (32).

Other comments

Zinc binds to proteins. It is required for the optimum function of 300 enzymes (33).

Essential element in mammalian metabolism (11).

Human dietary requirement for zinc 2-20 mg day⁻¹, depending on dietary intake of protein and phosphorus (34).

Severe zinc deficiency causes bulbous pustular dermatitis, diarrhoea, alopecia, mental disturbances and immune disorders. Moderate deficiency may cause growth retardation, ♂ hypergonadism, skin changes, poor appetite, mental lethargy, delayed wound healing and abnormal dark adaptation. Marginal deficiency is characterised by neurosensory changes, oligospermia and decreased testosterone in ♂, hyperammonaemia, decreased IL-2 production, decreased immune response, impaired neuropsychological functions and decreased ethanol clearance. Prevalence of zinc deficiency is high in populations consuming large quantities of cereal proteins containing high amounts of phytate (11).

Health effects of zinc reviewed (11).

A number of animal studies have suggested that zinc deficiency inhibits the growth of transplanted tumours, while high levels suppressed carcinogenesis induced by dimethylbenzanthracene in hamsters (11).

Reviews on human health effects, experimental toxicology, epidemiology and workplace experience listed (35).

Zinc (3.2, 6.5, and 13 mg l⁻¹) caused ultrastructural changes in plastids and heavy staining of the cell walls and mucilage of vegetative cells of *Ceranium ciliatum*. Carpospores remained unmodified (36).

References

1. Overall, N. C. et al *J. Fish Biol.* 1989, **35**(1), 27-36.
2. Scherer, E. et al *Water Res.* 1998, **32**(3), 924-929.
3. Hatakeyama, S. et al *Environ. Pollut.* 1989, **59**(4), 325-336.
4. Filov, V. A. et al (Eds.) *Harmful Chemical Substances* 1993, **17**, 189-209.
5. Wong, P. T. S. et al *Toxic Assess.* 1990, **5**(2), 167-177.
6. Van Gestel, C. A. M. et al *Environ. Toxicol. Chem.* 1997, **16**(6), 1177-1186.

7. Reed-Judkins, D. K. et al *Environ. Toxicol. Chem.* 1997, **16**(8), 1666-1676.
8. Kroetze, C. *Water Report* 1979, **9**, 5-6.
9. Martin, G. et al *Water Sci. Technol.* 1982, **14**, 781-794.
10. *Arch. Hyg.* 1910, **72**, 358.
11. Walsh, C. T. et al *Environ. Health Perspect.* 1994, **102**(Suppl. 2), 5-46.
12. NAS/NRC *Drinking Water and Health: The Contribution of Drinking Water to Mineral Nutrition in Humans* 1980, 265-403, National Academy of Science, Washington, DC, USA.
13. Mills, C. F. *Ann. Rev. Nutr.* 1985, **5**, 173-193.
14. Sandstroem, B. et al *J. Nutr.* 1987, **117**, 1898-1902.
15. Menard, M. P. et al *J. Nutr.* 1983, **113**, 1434-1442.
16. Wong, P. K. *Bull. Environ. Contam. Toxicol.* 1988, **40**(4), 597-603.
17. Fan, L. et al *Gongye Weisheng Yu Yihyebing* 1986, **12**(2), 77-80 (Ch.) (*Chem. Abstr.* **107**, 53901d).
18. Gukov, I. N. et al *Dopov. Akad. Nauk Ukr, RSR, Ser. B: Geol. Khim. Biol. Nauki* 1986, **12**, 61-63 (Ukrain.) (*Chem. Abstr.* **106**, 80134s).
19. Crofton, R. W. et al *Am. J. Clin. Nutr.* 1989, **50**, 141-144.
20. Chandra, R. K. *J. Am. Med. Assoc.* 1984, **252**, 1443-1446.
21. Cavallo, F. et al *Cancer* 1991, **67**, 738-745.
22. Schrauzer, G. N. et al *Bioinorg. Chem.* 1977, **7**, 23-24, 35-36.
23. van Rinsburg, S. J. et al *J. Natl. Cancer Inst.* 1981, **67**, 243-251.
24. Prasad, A. S. in Hsu, J. H. et al (Eds.) *The Biomedical Role of Trace Elements in Ageing* 1976, 15-33, Eckerd Coll., FL, USA.
25. Fosmine, G. J. *Am. J. Clin. Nutr.* 1990, **51**, 225-227.
26. Donaldson, J. et al *Can. J. Biochem.* 1971, **49**, 1217-1224.
27. Kress, Y. et al *Brain Res.* 1981, **220**, 139-149.
28. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
29. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
30. *J. Protect. Coat. Series* 1993, **10**(3), 77-79.
31. *Water and the Environment. The Implementation of European Community Directives on Pollution Caused by Certain Dangerous Substances Discharged into the Aquatic Environment* 1989, HMSO, London, UK.
32. Sandstead, H. H. in Prasad, A. S. (Ed.) *Clinical, Biochemical and Nutritional Aspects of Trace Elements* 1982, 83-101, Alan R. Wiss, New York, NY, USA.
33. Vallee, B. L. et al *Biochemistry* 1990, **29**, 5647-5659.
34. *Chemical Safety Data Sheets* 1992, 5, 277-281, The Royal Society of Chemistry, London, UK.
35. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
36. Diannelidis, B.-E. et al *Mar. Environ. Res.* 1997, **44**(2), 127-134

23 zinc acetate



$\text{C}_4\text{H}_6\text{O}_4\text{Zn}$

Mol. Wt. 183.48

CAS Registry No. 557-34-6

Synonyms dicarbomethoxy zinc; zinc diacetate

EINECS No. 209-170-2

RTECS No. AK 1500000

Uses Catalyst. Used in the treatment of Wilson's disease and in combination with erythromycin in the treatment of acne vulgaris. Has been used as an emetic. Analytical reagent. Mordant in dyeing. Manufacture of glazes for painting on porcelain.

Physical properties

M. Pt. 237°C (decomp.) **Specific gravity** 1.735

Solubility Water: 20%. Organic solvents: ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 2500 mg kg⁻¹ (1,2).

LD₅₀ intraperitoneal mouse 57 mg kg⁻¹ (3).

LD_{Lo} intravenous rabbit 5 mg kg⁻¹ (4).

Teratogenicity and reproductive effects

Lowest tissue dose, intravaginal rabbit single dose of 10.5 mg kg⁻¹ 1 day prior to mating reduced fertility index (5).

Subcutaneous ♂ rat, lowest tissue dose 80 mg kg⁻¹ affected spermatogenesis 1 day prior to mating (5).

Metabolism and toxicokinetics

In tumours during intestinal perfusion of zinc acetate, zinc absorption occurred throughout the entire small intestine. The jejunum had the highest rate of absorption, followed by the duodenum and then the ileum (6).

Irritancy

Dermal rabbit, guinea pig, mouse 20% aqueous solution day⁻¹ for 5 days caused irritation (7).

Dermal rabbit (24 hr) 500 mg caused mild irritation (dihydrate). 20 mg instilled into rabbit eye for 24 hr caused moderate irritation (dihydrate) (8).

Genotoxicity

Salmonella typhimurium TA80, TA100, TA1535, TA1537, TA1538 with and without activation negative (9).

In vitro mouse lymphoma L5178Y cells, tk⁺/tk⁻ forward mutation positive (9).

In vitro primary rat hepatocytes unscheduled DNA synthesis negative (9).

In vitro Chinese hamster ovary cells, chromosomal aberrations negative (9).

Other effects

Other adverse effects (human)

Zinc acetate and gluconate are reported to be less irritating to the gastro-intestinal tract than other forms of zinc (10).

Any other adverse effects

Intratracheal instillation rat single administration 5-200 µg Zn animal⁻¹ caused lung damage at ≥20 µg Zn doses (11).

Legislation

Limited under EC directive on Drinking Water Quality 80/778/EEC. Zinc: guide level 100 µg l⁻¹ at supply works, 5000 µg l⁻¹ after 12 hr contact with consumers' pipework (12).

Included in schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (13).

Other comments

Administration of zinc acetate offered protection against the carcinogenic effects of nickel and zinc (14,15).

References

1. Lewis, R. J. *Sax's Dangerous Properties of Industrial Materials* 8th ed., 1992, Van Nostrand Reinhold, New York, NY, USA.
2. Smyth, H. F. et al *Am. Ind. Hyg. Assoc. J.* 1969, **30**, 470.
3. *Toxicol. Appl. Pharmacol.* 1979, **49**, 41.
4. *Arch. Internal Med.* 1926, **37**, 641.
5. *Contraception* 1980, **22**, 659.
6. Lee, H. H. et al *Am. J. Physiol.* 1989, **256**, G87-G91.
7. Lansdown, A. B. G. *Food Chem. Toxicol.* 1991, **29**(1), 57-64.
8. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
9. Thompson, E. D. et al *Mutat. Res.* 1989, **223**(3), 267-272.

10. Solomons, N. W. in Prasad, A. S. (Ed.) *Essential and Toxic Trace Elements in Human Health and Disease* 1988, 509-518, Alan R. Liss, New York, NY, USA.
11. Kobayashi, E. et al *Eisei Kagaku* 1988, **34**(6), 524-530, (Japan) (*Chem. Abstr.* **110**, 1096983).
12. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
13. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
14. Kasprzak, K. S. et al *Toxicology* 1988, **52**, 253-262.
15. Waalkes, M. P. et al *Cancer Res.* 1989, **49**, 4282-4288

z4 zinc bromide



Br_2Zn

Mol. Wt. 225.20

CAS Registry No. 7699-45-8

Synonyms zinc dibromide

EINECS No. 231-718-4

RTECS No. ZH 1150000

Uses Used for the mild cleavage of the β -methoxyethoxymethyl moiety; an hydroxyl protecting group (1).
Catalyst. Electrolyte. Manufacture of silver bromide emulsions for photography. Shielding viewing windows for nuclear reactions.

Physical properties

M. Pt. 394°C B. Pt. 697°C Specific gravity 4.201 at 25°C with respect to water at 4°C

Solubility Water: 1 g dissolves in 0.25 ml water. Organic solvents: acetone, diethyl ether, ethanol

Mammalian & avian toxicity

Irritancy

Causes eyes and skin irritation (species unspecified) (2).

Genotoxicity

In vitro rat ascites tumour cells, altered cell morphology, including chromosomal effects (3).

Other effects

Other adverse effects (human)

Ingestion of large doses can cause severe abdominal pain, violent vomiting, shock and collapse. Doses of <75 mg may be fatal (2).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC, Zinc: guide level 100 $\mu\text{g l}^{-1}$ at supply works, 5000 $\mu\text{g l}^{-1}$ after 12 hr contact with consumers' pipework (4).

References

1. *Tetrahedron Lett.* 1976, 809.
2. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3629, Sigma-Aldrich, Milwaukee, WI, USA.
3. Kimura, I. et al *Gann* 1963, **54**, 155-161.
4. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

z5 zinc carbonate



CO_3Zn

Mol. Wt. 125.40

CAS Registry No. 3486-35-9

Synonyms carbamic acid, zinc salt (1:1); Calamine; C.I. 77950; natural smithsonite; Zinespar

EINECS No. 222-477-6

RTECS No. FG 3375000

Uses Corrosion inhibitor. In deodorants. Filler for plastics. Fireproofing agent. Catalyst. In the treatment of skin disorders (component of Calamine). Pigment. Dietary supplement.

Occurrence In the minerals smithsonite and zincspar. Forms on surface of metallic zinc during atmospheric corrosion.

Physical properties

M. Pt. 140°C (decomp.) **Specific gravity** 4.398

Solubility Water: 10 mg l⁻¹ at 15°C

Mammalian & avian toxicity

Sub-acute and sub-chronic data

Oral weanling pig, 0.1-0.8% diet for 42 days depressed growth rates and food intake and caused arthritis and extensive haemorrhages in the axillary region. Some animals died within 42 days; autopsy revealed gastritis, enteritis, and haemorrhages to the lymph nodes, internal organs and brain ventricles. Doses of 0.05% diet did not produce toxic effects (1).

Carcinogenicity and chronic effects

A study of carcinogenicity in mice, the incidence of pulmonary adenomas following intratracheal administration was 3/12 in zinc carbonate treated mice, 7/18 in untreated mice, and 31/62 in zinc chromate treated mice (doses unspecified) (2,3).

Teratogenicity and reproductive effects

Oral mouse, lowest toxic dose, single administration of 2800 mg kg⁻¹ 14 days after giving birth, developmental effects to skin and skin appendages (4).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Zinc: guide level 100 µg l⁻¹ at supply works, 5000 µg l⁻¹ after 12 hr contact with consumers' pipework (5).

References

1. Brink, H. et al *J. Anim. Sci.* 1959, **78**, 836-842.
2. *IARC Monograph* 1990, **49**, 122.
3. Steffee, C. H. et al *Arch. Environ. Health* 1965, **11**, 66-75.
4. Berry, C. L. (Ed.) *Teratology* 1975, **83**, Springer Verlag, New York, NY, USA.
5. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

z6 zinc chloride



Cl_2Zn

Mol. Wt. 136.30

CAS Registry No. 7646-85-7

Synonyms butter of zinc; zinc dichloride; zinc muriate

EINECS No. 231-592-0

RTECS No. ZH 1400000

Uses In dentifrices. Treatment of skin complaints. Deodorant. Dietary supplement. Flux in plating, soldering and welding. Pigment. In wood preservatives. Astringent.

Occurrence Formed during ignition of zinc oxide/hexachloroethane incendiary devices (1).

Physical properties

M. Pt. 293°C B. Pt. 732°C Specific gravity 2.907 at 25°C Volatility v.p. 1 mmHg at 428°C

Solubility Water: 4320 g l⁻¹ at 25°C. Organic solvents: acetone, ethanol, glycerol

Occupational exposure

FR-VME 1 mg m⁻³ (fume)

SE-LEVL 1 mg m⁻³ (respirable dust)

UK-LTEL 1 mg m⁻³ (fume)

UK-STEL 2 mg m⁻³ (fume)

US-TWA 1 mg m⁻³ (fume)

US-STEL 2 mg m⁻³ (fume)

UN No. 1840 (solution)

UN No. 2331 (anhydrous) HAZCHEM Code 2X Conveyance classification corrosive substance

Supply classification corrosive

Risk phrases Causes burns (R34)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep container tightly closed and dry – After contact with skin, wash immediately with plenty of water – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S7/8, S28, S45)

Ecotoxicity

Fish toxicity

Lethal to fathead minnow at <80 mg l⁻¹ as zinc (exposure unspecified) (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 350 mg kg⁻¹ (3).

LC_{Lo} (10 min) inhalation rat 2000 mg m⁻³ (4).

LD₅₀ intraperitoneal mouse 24 mg kg⁻¹ (5).

LD₆₀₋₉₀ intravenous rat 30 mg kg⁻¹ (6).

Teratogenicity and reproductive effects

Intravaginal rabbit, lowest toxic dose 30,000 mg kg⁻¹ 1 day prior to mating caused reduced fertility (7).

Metabolism and toxicokinetics

Plasma levels of zinc returned to normal or above in pregnant rats on a zinc-deficient diet following 8 or 24 dermal applications of zinc chloride in corn oil (8).

Irritancy

Dermal rabbit, guinea pig, mouse 1% aqueous solution day⁻¹ for 5 days caused severe irritation (9).

Sensitisation

Clearly sensitising in humans. Cases of allergic dermatitis involving extensive body areas have been reported (10).

However, allergic reactions to this caustic salt are reported to be rare (8).
95 patients were epicutaneous patch tested for sensitivity of dental alloys. 1.1% of patients tested positive for zinc allergy (11).

Genotoxicity

Escherichia coli WP2 (λ) Microscreen assay positive (12).
Salmonella typhimurium TA98, TA100, TA102, TA1537, TA 2637 negative. When tested in combination with 9-aminoacridine, the mutation rate was higher than that for *o*-aminoacridine alone (13).
In vitro human lymphocytes, chromosomal aberrations positive (14).
In vitro mouse lymphoma L5178Y cells tk⁺/tk⁻ assay negative (15).
In vitro human lymphocytes, low concentrations stimulated DNA synthesis, high concentrations inhibited DNA synthesis (16).
In vivo mouse bone marrow cells, chromosomal aberrations were induced in calcium-deficient mice but not in normal calcium-supplemented mice (17).

Other effects

Other adverse effects (human)

Accidental ingestion of ~75 g of a liquid zinc chloride solution caused local caustic effects including erosion of pharynx and oesophagus. Other symptoms were burning pain in the mouth, with nausea, vomiting and abdominal pain. In 1 subject, possible effects on the pancreas were indicated by elevated serum amylase and fasting blood-sugar levels (18).
Inhalation exposure to 600 mg m⁻³ for 5 hr resulted in "metal fume fever" characterised by irritation to the lungs, coughing, fatigue, shortness of breath and a metallic taste in the mouth (8).
Exposure to ~10 g m⁻³ near smoke incendiary devices was fatal to 10/34 treated patients (19).

Any other adverse effects

Intratracheal instillation rat 2.5 mg kg⁻¹ caused some pulmonary oedema, alveolitis and, at a later stage, some fibrosis (20).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Zinc: guide level 100 μ g l⁻¹ at supply works, 5000 μ g l⁻¹ after 12 hr contact with consumers' pipework. Chlorides: guide level 25 mg l⁻¹ (21).
UK maximum admissible concentration in drinking water, chloride 400 mg l⁻¹ (12-monthly average) (22).

Other comments

Preparations almost always contain some oxychloride (23).
Reviews on human health effects, experimental toxicology, physico-chemical properties listed (24,25).

References

1. Richards, R. J. et al *Toxicology* 1989, **54**(1), 79-88.
2. Erten, M. J. et al *Proc. Ind. Waste Conf.* 1988, **43rd**, 617-629.
3. Calvery, H. O. *Food Res.* 1942, **7**, 313-331.
4. Karlsson, N. et al *Arch. Toxicol.* 1986, **59**, 160-166.
5. Williams, M. W. et al *Toxicol. Appl. Pharmacol.* 1982, **63**, 461-469.
6. Bruner, *Fed. Proc.* 1950, **9**, 260.
7. *Contraception* 1980, **22**, 659-672.
8. Rom, W. N. *Environmental and Occupational Medicine* 1983, Little Brown & Co, Boston, MA, USA.
9. Lansdown, A. B. G. *Food Chem. Toxicol.* 1991, **29**(1), 57-64.
10. Filov, V. A. et al (Eds.) *Harmful Chemical Substances* 1993, **1**, 189-209, Ellis Horwood, New York, NY, USA.
11. Namikoshi, T. et al *J. Oral. Rehabil.* 1990, **17**(4), 377-381.
12. Rossman, T. G. et al *Mutat. Res.* 1991, **260**, 349-367.
13. Iychara, O. H. et al *Jpn. J. Genet.* 1987, **62**(2), 159-162.

14. DeKnudt, G. et al *Toxicology* 1978, **10**, 67-75.
15. Amacher, D. E. et al *Mutat. Res.* 1980, **78**, 279-288.
16. Nordlin, K. *Int. Arch. Allergy Appl. Immun.* 1985, **77**, 461-462.
17. DeKnudt, G. et al *Mutat. Res.* 1979, **68**, 163-168.
18. Chobanian, S. J. *Ann. Emerg. Med.* 1981, **10**, 91-93.
19. Evans, E. H. *Lancet* 1945, **2**, 368-370.
20. Brown, R. F. R. et al *Environ. Health Perspect.* 1990, **85**, 81-87.
21. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
22. *S.I. 1989 No. 1147. The Water Supply (Water Quality) Regulations* 1989, HMSO, London, UK.
23. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
24. Walsh, C. T. et al *Environ. Health Perspect.* 1994, **102**(Suppl. 2), 5-46.
25. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

27 zinc chromate



CrO₄Zn

Mol. Wt. 181.38

CAS Registry No. 13530-65-9

Synonyms Buttercup Yellow; chromic acid, zinc salt (1); chromium zinc oxide; C.I. 77955; C.I. Pigment Yellow 36; Citron Yellow; zinc chromate(vi) hydroxide; zinc chrome yellow; zinc chromium yellow; zinc hydroxychromate

EINECS No. 236-878-9

RTECS No. GB 3290000

Uses Corrosion inhibitor in primer paints. Pigment.

Physical properties

M. Pt. 316°C **Specific gravity** 3.40

Solubility Water: 31 g l⁻¹

Occupational exposure

FR-VME 0.05 mg m⁻³ (as Cr)

JP-OEL 0.05 mg m⁻³ (as Cr)

SE-LEVL 0.02 mg m⁻³ (as Cr)

UK-LTEL MEL 0.05 mg m⁻³ (as Cr)

US-TWA 0.01 mg m⁻³ (as Cr)

Supply classification toxic

Supply classification dangerous for the environment

Risk phrases May cause cancer – Harmful if swallowed – May cause sensitisation by skin contact – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R45, R22, R43, R50/53)

Safety phrases Avoid exposure – obtain special instruction before use – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S53, S45, S60, S61)

Mammalian & avian toxicity

Acute data

LD_{Lo} intravenous mouse 30 mg kg⁻¹ (1).

Carcinogenicity and chronic effects

Sufficient evidence for carcinogenicity to humans and animals, IARC classification group 1 (chromium(vi) compounds) (2).

Intratracheal instillation mouse, 0.03 ml of a 0.2% saline suspension of basic potassium zinc chromate (K₂O₄ZnO₄CrO₃3H₂O) at 6 wk intervals for 30 wk, then observed for life. No pulmonary carcinoma was found. Pulmonary adenomas occurred in 31/62 treated and 7/18 untreated mice and 3/12 zinc carbonate treated mice (3).

Intrabronchial rat (2 yr) 2 mg implanted in a stainless steel mesh. Bronchial carcinomas occurred in 8/200 treated animals, compared with 0/100 cholesterol treated controls, 2/100 treated with chromium trioxide, 1/100 treated with sodium dichromate, and 25/100 among positive controls treated with calcium chromate (4).

Intramuscular implant rat, basic zinc chromate (dose unspecified) induced implantation-site tumours (type unspecified) in 16/34 animals in 2 yr compared with 0/32 vehicle controls 0/33 sodium dichromate treated rats and 17/66 calcium chromate treated rats. Survival rates in these groups after 1 yr were 16/34, 30/32, 25/33 and 44/66, respectively (5)

Metabolism and toxicokinetics

Inhalation rats 6-11 mg m⁻³ caused a five-fold increase in blood chromium levels after 100 minutes exposure. Blood chromium levels fell by < 50% during the 3 days after exposure; after 18 and 37 days 20% and 9% respectively, of the initial concentration remained (6).

Genotoxicity

Salmonella typhimurium TA100 with and without metabolic activation positive (7).

In vitro Chinese hamster ovary cells, sister chromatid exchanges and chromosomal aberrations positive (7).

In vitro Chinese hamster V79 cells HPRT assay positive (8).

Similar results were obtained for basic zinc chromate (7,9,10).

Other effects

Other adverse effects (human)

A significant increase in risk of lung cancer was identified in 7/9 epidemiological studies among zinc and lead chromate pigment workers (2).

Reported to cause nasal ulceration and dermatitis in exposed workers (11).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Zinc: guide level 100 µg l⁻¹ at supply works, 5000 µg l⁻¹ after 12 hr contact with consumers pipework. Chromium: maximum admissible concentration 50 µg l⁻¹ (12).

The UK Industrial Injuries Advisory Council has extended its list of jobs covered for lung cancer compensation to include workers exposed to zinc chromate (13).

Other comments

Carcinogenicity, mutagenicity and mammalian toxicity of chromium compounds reviewed (2,13,14).

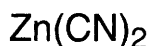
Decomposes at 540°C to ZnCr₂O₄ and ZnO.

References

1. *Air Quality Monograph* 1970, 70-15.
2. *IARC Monograph* 1990, 49, 49-256.
3. Steffee, C. H. et al *Arch. Environ. Health* 1965, 11, 66-75.

4. Levy, L. S. et al *Br. J. Ind. Med.* 1986, **43**, 243-256.
5. Hueper, W. C. *Cancer Res.* 1961, **21**, 842-857.
6. Langard, S. et al *Acta Pharmacol. Toxicol.* 1978, **42**, 142-149.
7. Venier, P. et al *Mutat. Res.* 1985, **156**(3), 219-228.
8. Newbold, R. F. et al *Mutat. Res.* 1979, **67**, 55-63.
9. De Flora, J. *Carcinogenesis* 1981, **2**, 283-298.
10. Levis, A. G. et al *Br. J. Cancer* 1981, **44**, 219-235.
11. *Laboratory Hazard Data Sheet No. 76: Zinc and Zinc Compounds* 1988, The Royal Society of Chemistry, London, UK.
12. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
13. *Chemical Safety Data Sheets* 1991, **4b**, 261-264, The Royal Society of Chemistry, London, UK.
14. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

z8 zinc cyanide



$\text{C}_2\text{N}_2\text{Zn}$

Mol. Wt. 117.43

CAS Registry No. 557-21-1

Synonyms RCRA waste number P121; zinc dicyanide

EINECS No. 209-162-9

RTECS No. ZH 1575000

Uses Catalyst. Electroplating. Removal of ammonia from producer gas.

Physical properties

M. Pt. 800°C (decomp.) Specific gravity 1.852 at 20°C with respect to water at 4°C

Solubility Water: 5 mg l⁻¹ at 20°C

Occupational exposure

DE-MAK 5 mg m⁻³ (as CN) (inhalable dust fraction)

FR-VME 5 mg m⁻³ (as HCN)

SE-CEIL 5 mg m⁻³ (as CN)

UK-LTEL 5 mg m⁻³ (as CN)

UN No. 1713 Conveyance classification toxic substance

Supply classification very toxic

Risk phrases Very toxic by inhalation, in contact with skin and if swallowed – Contact with acids liberates very toxic gas (R26/27/28, R32)

Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep container tightly closed – After contact with skin, wash immediately with plenty of water – Do not empty into drains – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S7, S28, S29, S45)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) bluegill sunfish 0.18 mg l⁻¹ (1).

Invertebrate toxicity

LC₅₀ (48 hr) prawn 0.38 mg l⁻¹, crab 105 mg l⁻¹ (1).

Environmental fate

Degradation studies

Degraded by enzymes isolated from *Alcaligenes* strains 4009 and 4010 (2).

Abiotic removal

Cyanide removal effected by copper bearing ion exchange resin in the presence of reducing agent (sulfite, hydrosulfite, Fe²⁺ or hydrazine) (3).

Mammalian & avian toxicity

Acute data

LD₅₀ intraperitoneal rat 100 mg kg⁻¹ (4).

Other effects

Other adverse effects (human)

Has been reported to cause dermatitis (5).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Zinc: guide level 100 µg l⁻¹ at supply works, 5000 µg l⁻¹ after 12 hr contact with consumers' pipework. Cyanide: maximum admissible concentration 50 µg l⁻¹ (6).

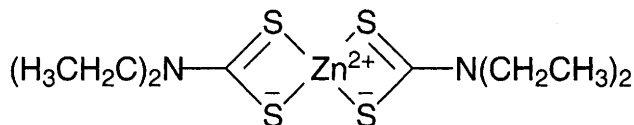
Other comments

Physical properties, mammalian and environmental toxicity reviewed (1).

References

1. *Dangerous Prop. Ind. Mater. Rep.* 1989, 9(5), 97-1041.
2. Invorsen, K. (Novo-Nordisk A/S) Eur. Pat. Appl. EP 349, 348 (Cl. C02F3/12) 3 Jan 1990.
3. Kato, I. (Kurita Water Ind. Ltd.) Jpn Kokai Tokkyo Koho JP 01 51, 191[89 51, 191] (Cl. C02F1/58) 27 Feb 1989, (*Chem. Abstr.* 111, 12126 a).
4. National Academy of Science *Review* 1953, 5, 28, National Research Council, Chem.-Biol. Coord. Center, Washington, DC, USA.
5. USDHEW/PHS *Occupational Diseases: A Guide to their Recognition* 1966, 239-24. Publ. No. 1094.
6. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

z9 zinc diethyldithiocarbamate



C₁₀H₂₀N₂S₄Zn

Mol. Wt. 361.94

CAS Registry No. 14324-55-1

Synonyms bis(diethyldithiocarbamate)zinc; Cynkotox; diethylcarbamic acid, zinc salt; ethylzimate; ethylziram; Valkacit LDA; zinc *N,N*-diethyldithiocarbamate

EINECS No. 238-270-9

RTECS No. ZH 0350000

Uses Antioxidant for rubbers. Vulcanisation accelerator. Antifouling agent.

Physical properties

M. Pt. 172-176°C **Specific gravity** 1.47 at 20°C with respect to water at 20°C
Solubility Organic solvents: benzene, carbon disulfide, chloroform

Occupational exposure

Supply classification harmful, dangerous for the environment

Risk phrases Harmful if swallowed – Irritating to eyes, respiratory system and skin – May cause sensitisation by skin contact – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment (R22, R36/37/38, R43, R50/53)

Safety phrases Keep out of reach of children (if sold to general public) – Avoid contact with the skin – Wear suitable gloves – This material and/or its container must be disposed of as hazardous waste – Avoid release to the environment. Refer to special instructions/safety data sheet (S2, S24, S37, S60, S61)

Ecotoxicity

Invertebrate toxicity

EC₅₀ (15 min) *Photobacterium phosphoreum* 1.7 ppm Microtox test (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, rabbit 570, 5200 mg kg⁻¹, respectively (2-5).

LD₅₀ subcutaneous rat, rabbit 600, 700 mg kg⁻¹, respectively (5).

LD₅₀ intraperitoneal mouse 140 mg kg⁻¹ (6).

Sub-acute and sub-chronic data

Oral rat 1000 mg kg⁻¹ day⁻¹ for 10 days caused degenerative changes to central nervous system and alterations to activity of various enzymes. Cerebral thiamine pyrophosphatase and acid phosphatase activities were increased, whereas acetylcholinesterase, butylcholinesterase and adenosine triphosphatase activities were decreased (4).

Teratogenicity and reproductive effects

Induced lethality and malformation when injected into chicken eggs at 1-10 mmol egg⁻¹. Most embryonic deaths occurred at stages 29-31 (7).

Irritancy

100 mg instilled into rabbit eye for 24 hr caused moderate irritation (2).

Genotoxicity

Salmonella typhimurium TA98, TA100 with and without metabolic activation positive (8).

Other effects

Other adverse effects (human)

Reported to cause urticaria in a young woman from contact with rubber gloves which incorporated zinc diethyldithiocarbamate. There were no signs of eczema (9).

Any other adverse effects

Zinc diethyldithiocarbamate was devoid of immunoenhancing influence on the response to T-cells mutagens, and it exerted a cytotoxic effect on spleen lymphocytes. These results are in contrast to enhancing activities of the sodium salt and known essential role of zinc in the functions of the immune system (species unspecified) (10).

Legislation

Limited under EC Directive on Drinking Water Quality 80/78/EEC. Zinc: guide level 100 µg l⁻¹ at supply works, 5000 µg after 12 hr contact with consumers' pipework (11).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration $0.1 \mu\text{g l}^{-1}$ (11).
Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (12).

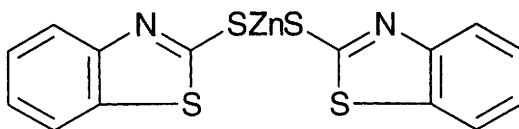
Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (13).
Exists in dimeric form in solid state.

References

1. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
2. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
3. *Ind. Med.* 1947, **16**, 473.
4. Kozink, M. B. *Acta Neuropathol. (Suppl.) (Berlin)* 1981, **7**, 56-58.
5. *Farmakol. Toksikol.* 1969, **32**, 356.
6. *Kobunshi Kako* 1977, **26**, 358.
7. Korhonen, A. et al *Teratog. Carcinog. Mutagen.* 1983, **3**(2), 163-175.
8. Yamaguchi, T. et al *Eisei Kagaku* 1991, **37**(1), 6-13 (Japan.) (*Chem. Abstr.* **115**, 2940y).
9. Helander, I. et al *Contact Dermatitis* 1983, **9**(4), 327-328.
10. Renoux, G. et al *Int. J. Immunopharmacol.* 1988, **10**(4), 489-493.
11. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
12. *S. I.* 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
13. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

z10 zinc 2-mercaptobenzothiazole



$\text{C}_{14}\text{H}_8\text{N}_2\text{S}_4\text{Zn}$

Mol. Wt. 397.89

CAS Registry No. 155-04-4

Synonyms 2(3*H*)-benzothiazolethione, zinc salt; bis(mercaptobenzothiazolato)zinc; Hermat Zn-MBT; Oscaf; Pennae ZT; Tisperse MB-58; Thiofax; VSAF GY-7; Vulkacit ZM; Zenite; zinc-2-benzothiazolethiolate

EINECS No. 205-840-3

RTECS No. DL 7000000

Uses Catalyst. Vulcanisation accelerator.

Physical properties

M. Pt. 177-178°C **Specific gravity** 1.7 at 25°C with respect to water at 4°C

Solubility Organic solvents: diethyl ether, ethanol

Mammalian & avian toxicity

Acute data

LD_{50} oral rat 540 mg kg^{-1} (1).

LD_{50} intraperitoneal mouse 200 mg kg^{-1} (2).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Zinc: guide level 100 µg l⁻¹ at supply works, 5000 µg l⁻¹ after 12 hr contact with consumers' pipework (3).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (4).

Other comments

Mercaptobenzothiazoles are reported to be irritants to skin and eye (species unspecified) (5,6).

References

1. *Technical Data Sheet* 9 Dec 1976, R.T. Vanderbilt Co. New York, NY, USA.
2. *NTIS Report AD 277-689*, Natl. Techn. Inf. Ser., Springfield, VA, USA.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
4. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
5. Grant, W. M. *Toxicology of the Eye* 2nd ed., 1974, 649, Charles, C. Thomas, Springfield, IL, USA.
6. Lefaux, R. *Practical Toxicology of Plastics* 1968, 177, CRC Press, Cleveland, OH, USA

211 zinc nitrate



N₂O₆Zn

Mol. Wt. 189.40

CAS Registry No. 7779-88-6

Synonyms Celloxan; zinc dinitrate

EINECS No. 231-943-8

RTECS No. ZH 4772000

Uses Catalyst. Corrosion inhibitor. A component of medicines used in the treatment of benign cervical lesions. Mordant in dyeing.

Physical properties

M. Pt. 36.4°C (hexahydrate) B. Pt. 105-131°C Specific gravity 2.065 (hexahydrate) at 14°C

Volatility v.p. 60 mmHg at 700°C

Solubility Water: ~200% w/w. Organic solvents: ethanol

Occupational exposure

UN No. 1514 HAZCHEM Code 1Y Conveyance classification oxidising substance

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) rainbow trout, sockeye salmon, brown trout, bluegill sunfish, guppy, fathead minnow 0.1-7.2 mg l⁻¹ (as zinc) (1).

Invertebrate toxicity

LD₅₀ (96 hr) *Tetrahymena pyriformis* 6.7 mg l⁻¹ (as zinc) (1).

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 240, 1600 mg kg⁻¹, respectively (2,3).

Irritancy

Dermal rabbit (24 hr) 500 mg caused severe irritation. 20 mg instilled into rabbit eye for 24 hr caused severe irritation (hexahydrate) (3).

Other effects

Any other adverse effects

In vitro dog tracheal epithelium 3 × 1mm solution reduced conductivity by 24%, but did not affect short circuit current. Sub-mucosal zinc nitrate inhibited short circuit current, but had little effect on conductivity (4).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Zinc: guide level 100 µg l⁻¹ at supply works, 5000 µg l⁻¹ after 12 hr contact with consumers' pipework. Nitrates: guide level 25 mg l⁻¹, maximum admissible concentration 50 mg l⁻¹ (5).

Other comments

Physical properties and environmental toxicity reviewed (1).

References

1. *Dangerous Prop. Ind. Mater. Rep.* 1988, 8(5), 101-110.
2. Spinidonova, V. S. et al *Gig. Tr. Prof. Zabol* 1986, 3.
3. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
4. Stutts, M. J. et al *Toxicol. Appl. Pharmacol.* 1982, 64(1), 147-84.
5. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

zinc oxide

ZnO

OZn

Mol. Wt. 81.39

CAS Registry No. 1314-13-2

Synonyms C.I. 77947; C.I. pigment white 4; Z-cote; Activox B; Electrox; Extrox; Microx; Canfelzo; Felzodox; Photozinc; Zinox

EINECS No. 215-222-5

RTECS No. ZH 4810000

Uses In cosmetics and sunscreens. In treatment of skin complaints. Astringent. In dental cements and ceramics. In single incendiary devices. Pigment. Temporary dental filling. Filler for plastics and rubbers.

Physical properties

M. Pt. 1975°C **B. Pt.** (Stable at 1720°C) **Specific gravity** 5.607 at 20°C with respect to water at 4°C
Solubility Water: 1.6 gm l⁻¹ at 28°C. Organic solvents: acetic acid

Occupational exposure

DE-MAK 1.5 mg m⁻³ (respirable fraction of aerosol) (fume)
FR-VME 1 mg m⁻³ (fume), 10 mg m⁻³ (dust)
JP-OEL 5 mg m⁻³ (fume)
SE-LEVL 5 mg m⁻³

UK-LTEL 5 mg m⁻³ (fume)

US-TWA 5 mg m⁻³ (fume); 10 mg m⁻³ (dust)

UK-STEL 10 mg m⁻³ (fume)

US-STEL 10 mg m⁻³ (fume)

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 8000 mg kg⁻¹ (1).

LC₅₀ inhalation mouse 2500 mg m⁻³ (exposure unspecified) (2).

LD₅₀ intraperitoneal rat 240 mg kg⁻¹ (3).

LD_{Lo} oral human 500 mg kg⁻¹ (4).

Inhalation rat, 11,380 mg m⁻³ zinc oxide/hexachloroethane smoke for 1 min caused pulmonary oedema, alveolitis and, at a later stage, some fibrosis (5).

Inhalation cat (15-45 min) 110-600 mg m⁻³ caused lethality and reduced body temperature in 15 min. After 45 min, complete prostration, tremor, respiratory distress, hypothermia and reduced erythrocyte counts were noted (6).

Inhalation guinea pig (3 hr) 25 mg m⁻³ caused severe pulmonary oedema (7).

Carcinogenicity and chronic effects

Inhalation rat, mice, guinea pig (18 month) 1.3, 12 or 120 mg zinc m⁻³ from zinc oxide/hexachloroethane smoke for 1 hr day⁻¹ 5 day wk⁻¹. Rats and mice received 100 daily exposures, but guinea pigs were exposed only to 15 doses because of high mortality. The most significant observation was an increase in alveologenic carcinoma in high-dose mice (8).

Teratogenicity and reproductive effects

Oral rat, lowest toxic dose 6800 mg kg⁻¹ day⁻¹ on dogs 1-22 of gestation, stillbirth and reduced growth occurred, but no anatomical malformations were observed (9).

Metabolism and toxicokinetics

Cats fed 70-140 mg kg⁻¹ day⁻¹ for 12-16 wk accumulated up to 480 mg kg⁻¹ in the pancreas, ~7 times the normal value (10).

Irritancy

Dermal rabbit, guinea pig, mouse 20% solution applied daily for 5 days caused moderate irritation (11).

Dermal rabbit (24 hr) 500 mg caused mild irritation. 500 mg instilled into rabbit eye caused mild irritation (12).

Genotoxicity

Salmonella typhimurium TA98, TA100 with and without metabolic activation negative (13).

In vitro Syrian hamster embryo cells, morphological transformations, unscheduled DNA synthesis and sister chromatid exchanges positive (14).

Other effects

Other adverse effects (human)

Solitary aspergillosis of the maxillary sinus in 29/30 patients was associated with zinc oxide from over-filled teeth (15).

Inhalation exposure to 5 mg m⁻³ for 8 hr caused clinical symptoms of metal fume fever in all four subjects (16).

Prolonged exposure to skin may produce severe dermatitis, known as "oxide pox" (17).

Bronchoalveolar lavage (BAL) cytokine concentrations were determined in 15 healthy volunteers 3 hr after inhaling zinc oxide fumes. These provided evidence for a pulmonary inflammatory response characterised by dose-dependent increases in BAL pro-inflammatory cytokine concentrations (18).

Any other adverse effects

In contrast to zinc chloride, which is formed on ignition of zinc oxide/hexachloroethene incendiary devices, zinc oxide did not induce pulmonary oedema in rats following intratracheal instillation (19).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Zinc: guide level 100 µg l⁻¹ at supply works, 500 µg l⁻¹ after 12 hr contact with consumers' pipework (20).

Other comments

Zinc oxide has been shown to accelerate the growth of *Aspergillus fumigatus* (15).

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (21).

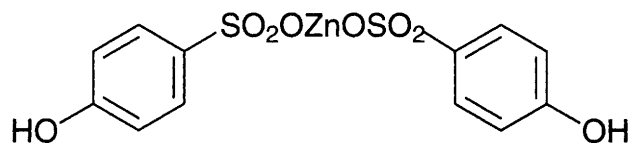
Health effects of zinc and zinc compounds reviewed (22).

Reaction with hexachloroethane in smoke bombs produces zinc chloride (22).

References

1. Gekkan Yakujii 1980, **22**, 291.
2. Gig. Sanit. 1986, **51**(4), 89.
3. Int. Polym. Sci. Technol. 1973, **3**, 93.
4. Zdrovookhraneni Kazakhstana 1978, **38**(9), 18.
5. Brown, R. F. R. et al *Environ. Health Perspect.* 1990, **85**, 81-87.
6. Filov, V. A. et al (Eds.) *Harmful Chemical Substances* 1993, **1**, 189-209.
7. Conner, M. et al *Toxicol. Appl. Pharmacol.* 1982, **20**, 434-442.
8. Marrs, T. C. et al *Arch. Toxicol.* 1988, **62**, 123-132.
9. J. Nutr. 1969, **98**, 303.
10. Scott, D. A. et al *Am. J. Physiol.* 1938, **121**, 253-260.
11. Lansdown, A. B. G. *Food Chem. Toxicol.* 1991, **29**(1), 57-64.
12. Marhold, J. V. *Sbornik Vysledku Toxikologickeho Vysetreni Latek A Pripravku* 1972, Prague, Czechoslovakia.
13. Yamaguchi, T. et al *Eisei Kagaku* 1991, **37**(1), 6-13 (Japan.) (*Chem. Abstr.* **107**, 822x).
14. Suzuki, H. *Shizaka* 1987, **74**(6), 1385-1403 (Japan.).
15. *Martindale: The Extra Pharmacopoeia* 31st ed., 1996, The Royal Pharmaceutical Society, London, UK.
16. Gordon, T. et al *Am. Ind. Hyg. Assoc. J.* 1992, **53**, 503-509.
17. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3631, Sigma-Aldrich, Milwaukee, WI, USA.
18. Kuschner, W. G. et al *Environ. Res.* 1997, **75**(1), 7-11.
19. Richards, R. J. et al *Toxicology* 1989, **54**(1), 79-88.
20. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
21. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
22. Walsh, C. T. et al *Environ. Health Perspect.* 1994, **102**(Suppl 2), 5-46.

z13 zinc *p*-phenolsulfonate



C₁₂H₁₀O₈S₂Zn

Mol. Wt. 411.73

CAS Registry No. 127-82-2

Synonyms benzosulfonic acid, zinc salt (2:1); zinc benzenesulfonate; zinc sulfocarbolate; *p*-hydroxy-benzenesulfonic acid, zinc salt; Phenozin

EINECS No. 204-867-8

RTECS No. DB 7120000

Uses In cosmetic and insecticide formulations. Astringent.

Physical properties

Solubility Water: 625 g l⁻¹ at 20°C. Organic solvents: ethanol

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse 1800, 3000 mg kg⁻¹, respectively (1).

LD₅₀ intraperitoneal mouse 225 mg kg⁻¹ (1).

Irritancy

3 mg instilled into rabbit eye caused moderate irritation (exposure unspecified) (1).

Other effects

Other adverse effects (human)

Contact with a 3% solution in an eye compress resulted in complete necrosis of both corneas in an infant (2).

Legislation

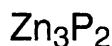
Limited under EC Directive on Drinking Water Quality 80/778/EEC. Zinc guide level 100 µg l⁻¹ at supply works, 5000 µg l⁻¹ after 12 hr contact with consumers' pipework (3).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (4).

References

1. *J. Am. Coll. Toxicol.* 1986, 5(5), 373.
2. Grant, W. M. *Toxicology of the Eye* 2nd ed., 1986, 990, Charles C. Thomas, Springfield, IL, USA.
3. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
4. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

Z14 zinc phosphide



P₂Zn₃

Mol. Wt. 258.12

CAS Registry No. 1314-84-7

Synonyms Arrex; Blue-ox; Gopha-Rid; Phosvin; Pollux; Ratol; Ridall; trizinc diphosphide; Zinc-Tox; ZP

EINECS No. 215-244-5

RTECS No. ZH 4900000

Uses Rodenticide.

Physical properties

M. Pt. 420°C (when heated in the absence of oxygen) **B. Pt.** 1100°C **Specific gravity** 4.55 at 13°C

Solubility Water: practically insoluble (decomposes slowly). Organic solvents: slightly in benzene, carbon disulfide

Occupational exposure

UN No. 1714 **Conveyance classification** substance which in contact with water emits flammable gas, toxic

Supply classification very toxic, highly flammable

Risk phrases Contact with water liberates toxic, extremely flammable gas – Very toxic if swallowed – Contact with acids liberates very toxic gas (R15/29, R28, R32)
Safety phrases Keep locked up and out of the reach of children (if sold to general public) – Keep in a cool well ventilated place away from oxidising agents and acids – Never add water to this product – Wear suitable protective clothing and gloves – In case of accident or if you feel unwell, seek medical advice immediately (show label where possible) (S1/2, S3/9/14, S30, S36/37, S45)

Ecotoxicity

Fish toxicity

LC₅₀ bluegill sunfish, rainbow trout 0.5-0.8 mg l⁻¹ (exposure unspecified) (1).

Invertebrate toxicity

LC₅₀ (24 hr) *Mesocyclops leuckarti* 0.2 mg l⁻¹ (2).

Mammalian & avian toxicity

Acute data

LD₅₀ pheasant, bobwhite quail, mallard duck 9, 13.5, 37.5 mg kg⁻¹, respectively (3).

LD₅₀ oral rat, mouse 12, 40 mg kg⁻¹ (4,5).

LD₅₀ dermal rabbit 2000-5000 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

LC₅₀ (5 day) oral mallard duck 1300 mg kg⁻¹ diet (6).

Oral ♀ rat, 0, 50, 200, 500 ppm diet for 13 wk. Death occurred in animals treated with 200 and 500 ppm and decreased body-weight gains were noted in all treated animals. A dose-dependent hair loss and decreased red blood cell count were also observed in all treated animals (7).

Metabolism and toxicokinetics

Following oral administration to rats, zinc phosphide reacts with stomach acids to liberate phosphine which enters the bloodstream (1).

Irritancy

Not irritating to skin and eyes (species unspecified) (1).

Other effects

Other adverse effects (human)

Inhalation of 300 ml phosphine m⁻³ for 1 hr has been reported to be fatal. No symptoms of chronic poisoning were observed (1).

Inhalation may cause lung irritation, pulmonary oedema, dilation of the heart and hyperaemia of the visceral organs. Chronic exposure may cause anaemia, bronchitis, and gastro-intestinal, visual, speech and motor disturbances (8).

Exposed workers have demonstrated neuropsychiatric syndromes such as anxiety, impotence and fatigue (9).

Any other adverse effects

Rodenticide action is through damage to the liver, kidneys and heart as the result of the absorption of phosphine formed in the stomach (1).

Legislation

WHO Class 1b (10).

EPA Toxicity Class 1 (formulation) (3).

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Zinc: guide level 100 µg l⁻¹ at supply works, 5000 µg l⁻¹ after 12 hr contact with consumers' pipework. Phosphorus: guide level 400 µg l⁻¹; maximum admissible concentration 5000 mg kg l⁻¹ (as P₂O₅). Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (11).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (12).

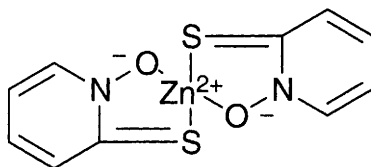
Other comments

Reviews on physical properties, uses, mammalian toxicity and health precautions are listed (11-14).

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. Deshmukh, P. B. et al *Pollut. Res.* 1989, 8(4), 163-165.
3. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
4. *Malasian Agric. J.* 1979, 52(2), 166.
5. *Yakkyoku* 1980, 31, 1247.
6. Hill, E. F. et al *Lethal Dietary Toxicities of Environmental Pollutants to Birds* 1975, US Fish and Wildlife Service, Report Wildlife No. 191, Washington, DC, USA.
7. Bai, K. M. et al *Indian J. Exp. Biol.* 1980, 18(8), 854-857.
8. *Chemical Safety Data Sheets* 1991, 4a, 265-268, The Royal Society of Chemistry, London, UK.
9. Amr, M. M. et al *Environ. Res.* 1997, 73(1/2), 200-206.
10. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
11. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
12. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
13. *Dangerous Prop. Ind. Mater. Rep.* 1985, 5, 103-106.
14. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

z15 zinc pyrithione



$C_{10}H_8N_2O_2S_2Zn$

Mol. Wt. 317.71

CAS Registry No. 13463-41-7

Synonyms bis(1-hydroxy-2(1H)-pyridinethionato)zinc; bis(2-pyridylthio)zinc 1,1'-dioxide; omadine zinc; pyrithione zinc; Vancide P; zinc omadine; zinc polyanemine; zinc PT; ZPT; zinc pyridinethione; zinc pyrion

EINECS No. 236-671-3

RTECS No. ZH 0950000

Uses Biocide used in anti-dandruff shampoos. Fungicide.

Physical properties

M. Pt. 262°C **Specific gravity** 1.782 at 25°C

Solubility Organic solvents: chloroform, dimethylformamide, dimethyl sulfoxide

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat, mouse, dog 160-600 mg kg⁻¹ (1,2).

LD₅₀ dermal rabbit 100 mg kg⁻¹ (3).

LD₅₀ subcutaneous mouse 730 mg kg⁻¹ (1).

LD₅₀ intraperitoneal mouse 27 mg kg⁻¹ (4).

LD_{Lo} intravenous rabbit, dog, monkey 10-25 mg kg⁻¹ (5).

Teratogenicity and reproductive effects

A 48% aqueous slurry was administered topically to rats (without prevention of ingestion through grooming) from 8 wk prior to mating to day 15 of gestation, at 2.5, 7.5 or 15 mg kg⁻¹ day⁻¹. No adverse effects on growth, pathology or conception (parents) or on viability, post-weaning growth or pathology in the neonates were noted. Treated ♀ were mated a second time and given 7 or 15 mg kg⁻¹ day⁻¹ in corn oil on days 6-15 of gestation. Reduced weight-gain was noted and 50% of animals exhibited paralysis. Foetal weights were significantly reduced and the incidence of rib defects significantly increased (6).

Irritancy

Dermal rabbit, guinea pig, mouse 20% suspension applied daily for 5 days caused moderate irritation (7). 1 mg instilled into rabbit eye for 48 hr caused irritation (8).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537 with and without metabolic activation negative (9).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (10).

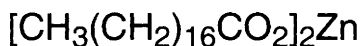
Limited under EC Directive on Drinking Water Quality 80/778/EEC. Zinc: guide level 100 µg l⁻¹ at supply works, 5000 µg l⁻¹ after 12 hr contact with consumers' pipework (10).

Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (11).

References

1. *Clin. Toxicol.* 1978, **13**, 1.
2. *Toxicol. Ann.* 1979, **3**, 1.
3. *Yakkyoku* 1981, **32**, 965.
4. *Oyo Yakuri* 1974, **8**, 1067.
5. *Toxicol. Appl. Pharmacol.* 1966, **9**, 269.
6. Nolen, G. A. et al *Food Cosmet. Toxicol.* 1979, **17**(6), 639.
7. Lansdown, A. B. G. *Food Chem. Toxicol.* 1991, **29**(1), 57-64.
8. *J. Assoc. Official Analyt. Chem.* 1973, **56**, 905.
9. Zeiger, E. et al *Environ. Mutagen.* 1987, **9**(Suppl. 9), 1-109.
10. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
11. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK

Z16 zinc stearate



C₃₆H₇₀O₄Zn

Mol. Wt. 632.34

CAS Registry No. 557-05-1

Synonyms dibasic zinc stearate; octadecanoic acid, zinc salt; stearic acid, zinc salt; zinc distearate; zinc octadecanoate

EINECS No. 209-151-9

RTECS No. ZH 5200000

Uses Cross-linking catalyst. In electrophotographic developers. Heat stabiliser for polymers. Lubricant for powder blends. Plasticiser. In cosmetics. Dietary supplement.

Physical properties

M. Pt. 128-130°C Flash point 355°C (open cup) Specific gravity 1.095
Solubility Organic solvents: benzene

Occupational exposure

FR-VME 10 mg m⁻³
UK-LTEL 10 mg m⁻³ (total inhalable dust); 4 mg m⁻³ (respirable dust) UK-STEL 20 mg m⁻³ (total inhalable dust)
US-TWA 10 mg m⁻³

Ecotoxicity

Fish toxicity
Not toxic to bluegill sunfish because of insolubility (1).

Mammalian & avian toxicity

Acute data
LD_{Lo} intratracheal rat 250 mg kg⁻¹ (2).

Other effects

Other adverse effects (human)
Aspiration of powder has produced acute fatal pneumonitis in infants; lesions resembled those from talc but were generally more severe (3).
Dust inhalation from occupational exposure in the rubber industry was reported to cause no adverse effects (4).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Zinc guide level 100 µg l⁻¹ at supply works, 5000 µg l⁻¹ after 12 hr contact with consumers' pipework (5).
Included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (6).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (7).
Autoignition temperature 411°C.

References

1. Verschueren, K. *Handbooks of Environmental Data on Organic Chemicals* 2nd ed., 1983, 1200, Van Nostrand Reinhold, New York, NY, USA.
2. *Br. J. Ind. Med.* 1958, 15, 130.
3. Gosselin, R. E. et al *Clinical Toxicology of Commercial Products* 5th ed., 1984, II-143, Williams & Wilkins, Baltimore, MD, USA.
4. *Documentation of Threshold Limit Values and Biological Exposure Indices* 5th ed., 1986, 646, American Conference of Governmental Hygienists, Cincinnati, OH, USA.
5. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
6. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
7. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuysse (Bte 6), B-1160 Brussels, Belgium

217 zinc sulfate



O₄SZn

Mol. Wt. 161.45

CAS Registry No. 7733-02-0

Synonyms Barazen; bufopto zinc sulfate; Op-thal-zin; sulfuric acid, zinc salt (1:1); Verazinc white copperas; White vitriol; zinc vitriol

EINECS No. 231-793-3

RTECS No. ZH 5260000

Uses Catalyst. Corrosion inhibitor. Deodorant. Electrolyte. In fertilisers and animal feeds. In wood preservatives. Pigments in paints. In the treatment of Wilson's disease.

Physical properties

M. Pt. decomposes at >500°C **Specific gravity** 1.957 (heptahydrate) at 25°C with respect to water at 4°C

Solubility Water: 965 g l⁻¹ at 20°C (heptahydrate). Organic solvents: ethanol, methanol

Occupational exposure

Supply classification irritant

Risk phrases Irritating to eyes and skin (R36/38)

Safety phrases Keep out of reach of children (if sold to general public) – Do not breathe dust – Avoid contact with the eyes (S2, S22, S25)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) cichlid 13 ppm Zn (as ZnSO₄) (1).

Lethal in fathead minnow at <10 mg l⁻¹ as zinc (exposure unspecified) (2).

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse 57 mg kg⁻¹ (3).

LD₅₀ oral rat 2900 mg kg⁻¹ (4).

LD₅₀ intraperitoneal mouse 72 mg kg⁻¹ (5).

LD_{L0} subcutaneous mouse, dog, rat 2, 78, 330 mg kg⁻¹ (6,7).

LD_{L0} intravenous rat, dog 50, 66 mg kg⁻¹, respectively (7).

Sub-acute and sub-chronic data

Oral rat 5.5 mg kg⁻¹ as zinc day⁻¹ for 3 days, bone zinc content, calcium content and alkaline phosphatase activity was raised. Bone DNA content was not significantly affected (8).

Oral mouse (13 wk) 150-3900 mg kg⁻¹ day⁻¹. Doses ≥1500 mg kg⁻¹ caused ulcers in the forestomach (9).

Teratogenicity and reproductive effects

Subcutaneous hamster, lowest toxic dose, single injection of 15 mg kg⁻¹ on day 8 of gestation was neither lethal to embryo nor teratogenic. A 30 mg Zn kg⁻¹ dose increased the frequency of oedematous fetuses (10).

Irritancy

Dermal rabbit, guinea pig, mouse 1% aqueous solution applied daily for 5 days caused moderate irritation (11).

420 µg instilled into rabbit eye caused moderate irritation (exposure unspecified) (12).

Genotoxicity

Salmonella typhimurium TA97, TA102 with and without metabolic activation negative (13,14).

Drosophila melanogaster sex-linked recessive lethal assay negative (15).

In vitro rat ascites tumour cells, altered cell morphology, including chromosomal effects (16).

In vitro human lymphocytes, unscheduled DNA synthesis positive (17).

In vivo mouse bone marrow cells, micronucleus assay negative (15).

Other effects

Other adverse effects (human)

Oral human, 25 mg as Zn $4 \times \text{day}^{-1}$ for 3-6 months. Only 1/80 subjects experienced mild diarrhoea as the only gastro-intestinal disturbance. In contrast 50 mg as zinc sulfate $3 \times \text{day}^{-1}$ for 6 wk caused gastro-intestinal disturbances in 26/47 subjects (18,19).

Any other adverse effects

In vitro guinea pig aortic smooth muscle $1.6\text{--}16 \text{ mg l}^{-1}$ inhibited contractions induced by potassium chloride, calcium chloride and norepinephrine. This effect may result from the antagonistic effect on transmembrane Ca^{2+} channels (20).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Zinc: guide level $100 \mu\text{g l}^{-1}$ at supply works, $5000 \mu\text{g l}^{-1}$ after 12 hr contact with consumers' pipework. Sulfates: guide level 25 mg l^{-1} , maximum admissible concentration 250 mg l^{-1} (21).

Other comments

Health effects and zinc and zinc compounds reviewed (22).

References

1. Gaikwad, S. A. *Pollut. Res.* 1989, **8**(1), 33-35.
2. Erten, M. J. et al *Proc. Ind. Waste Conf.* 1988, **43rd**, 617-629.
3. *Int. Polymer Sci. Technol.* 1976, **3**, 93.
4. *Toxicol. Eur. Res.* 1978, **1**, 371.
5. *C. R. Acad. Sci.* 1963, **256**, 1043.
6. *Environ. Qual. Saf.* 1975, **1**(Suppl.), 1.
7. *Tokyo Joshi Ika Daigaku Zasshi* 1978, **48**, 313.
8. Yamaguchi, M. et al *Res. Exp. Med.* 1990, **190**(2), 105-110.
9. Maita, K. et al *J. Pestic. Sci.* 1981, **6**, 327-336.
10. Gale, T. F. *Environ. Res.* 1984, **35**(2), 405-412.
11. Lansdown, A. B. G. *Food Chem. Toxicol.* 1991, **29**(1), 57-64.
12. *J. Am. Pharm. Soc.* 1956, **45**, 474.
13. Fujita, H. et al *Kenkyu Nenpo- Tokyo-toritsu Eisei Kenkyusher* 1988, (39), 343-350 (Japan.) (*Chem. Abstr.* **110**, 230308a).
14. Marzin, D. R. et al *Mutat. Res.* 1985, **155**, 49-51.
15. Gock, E. et al *Mutat. Res.* 1981, **90**, 91-109.
16. Kimura, I. et al *Cann* 1963, **54**, 155-161.
17. Zheng, X. et al *Gongye Weishang Yu Zhiyebing* 1990, **16**(1), 27-30 (Ch.) (*Chem. Abstr.* **113**, 167202f).
18. Henkin, R. I. et al *Am. J. Med. Sci.* 1976, **272**, 285-299.
19. Sanaman, S. et al *Med. J. Austr.* 1987, **146**, 246-249.
20. Ma, X. et al *Yaoxue Xuebao* 1989, **24**(10), 786-788 (Ch.) (*Chem. Abstr.* **112**, 48483t).
21. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
22. Walsh, C. T. et al *Environ. Health Perspect.* 1994, **102**(Suppl. 2), 5-46.

C₄H₆N₂S₄Zn

Mol. Wt. 275.76

CAS Registry No. 12122-67-7

Synonyms ethylenebis(dithiocarbamate)zinc; [[1,2-ethanediy]bis[carbamodithioato]](2-)]zinc; zinc ethylenebis(dithiocarbamate) (polymeric)

EINECS No. 235-180-1

RTECS No. ZH 3325000

Uses Fungicide.

Physical properties

M. Pt. 157°C (decomp. without melting) **Flash point** 90°C **Partition coefficient** log P_{ow} ≤1.301 (1)

Volatility v.p. <7.5 × 10⁻⁸ mmHg at 20°C

Solubility Water: ~10 mg l⁻¹ at 20°C. Organic solvents: carbon disulfide, pyridine

Occupational exposure

Supply classification irritant

Risk phrases Irritating to the respiratory system – May cause sensitisation by skin contact (R37, R43)

Safety phrases Keep out of reach of children (if sold to general public) – Keep container dry – Avoid contact with skin and eyes – If swallowed seek medical advice immediately and show this container or label (S2, S8, S24/25, S46)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) harlequin fish 250 mg l⁻¹ (70% formulated product) (2).

LC₅₀ (96 hr) guppy 7.2 mg l⁻¹ (3).

LC₅₀ perch, roach 2, 6-8 mg l⁻¹, respectively (duration unspecified) (1).

Invertebrate toxicity

EC₅₀ (96 hr) *Chlorella pyrenoidosa* 1.8 mg l⁻¹ (3).

LC₅₀ (48 hr) *Daphnia magna* 0.97 mg l⁻¹ (3).

EC₅₀ (30 min) *Photobacterium phosphoreum* 2.1 ppm, Microtox test (4).

Not toxic to bees (5).

Bioaccumulation

Bioconcentration factor in golden ide (*Leuciscus idus melanotus*) after 3 days was <10; in the algae *Chlorella fuscavar* and *Vacuolata* after 1 day was 170 (6).

Environmental fate

Nitrification inhibition

Minimum inhibitory concentration (3 hr) for *Nitrosomonas* sp. and *Nitrobacter* sp. 18 mg l⁻¹ (3).

Completely inhibited *Nitrosomonas* sp. at 1 mg l⁻¹ in water, and at 5 mg kg⁻¹ in soil (7).

Degradation studies

In a screening test using activated sludge inoculum, 1.1% of the applied zineb was degraded in 5 days. Zinc is released from the molecule by soil microorganisms to a considerable extent (8,9).

In the atmosphere, zineb exists as dust or as an aerosol and is lost by gravitational settling. t_{1/2} in an experimental spray chamber for ¹⁴C-zineb and the ethylenediamine derivative were 11 and 14 days, respectively (10).

Abiotic removal

Ozonation was effective in reducing levels of ≤600 µg l⁻¹ in wastewater to <0.1 µg l⁻¹ at doses of 1.5-2.3 mg l⁻¹ at pH 8.0-8.5. Remaining traces were adsorbed onto activated carbon (11).

When adsorbed onto silica gel and irradiated for 17 hr at >290 nm, 5.1% was degraded (6).

Zineb is unstable in aqueous solutions producing ethylenethiourea, 5,6-dihydro-3*H*-imidazo-1,2, 4-dithiazole-3-thione, ethylenediamine, ethylenediisothiocyanate, sulfur, carbon disulfide and hydrogen sulfide. An increase in pH increases the formation of ethylenethiourea (8).

Adsorption and retention

Calculated K_{oc} 1230 indicated that zineb will undergo appreciable adsorption to soil (12).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird, starling >100 mg kg⁻¹ (13).

LD₅₀ oral rat 1850 mg kg⁻¹ (14).

LD₅₀ oral mouse 7600 mg kg⁻¹ (15).

LC_{Lo} (4 hr) inhalation rat 800 mg m⁻³ (16).

LD₅₀ dermal rat >6000 mg kg⁻¹ (1).

Sub-acute and sub-chronic data

Inhalation rat, 2, 10, 50, 110 mg m⁻³ (exposure and duration unspecified) caused toxicological changes and irritation in the lungs and trachea. ¹³¹I uptake and thyroid activity were increased. A decrease in fertility, destruction of Leydig cells and injury of theca interna, granulosa and interstitium were also reported (17).

Carcinogenicity and chronic effects

No adequate data for evaluation of carcinogenicity to humans, insufficient evidence of carcinogenicity to animals, IARC classification group 3 (18).

Oral rat (2 yr) 5 or 10 g kg⁻¹ diet. 5 and 10 g kg⁻¹ doses caused mortality in ♀ rats. A goitrogenic effect was observed at all doses (19).

Oral dog (1 yr) 10 g kg⁻¹ diet caused hyperplasia of the thyroid (19).

Gavage mouse (18 month) 460 mg kg⁻¹ day⁻¹ from 7 days of age for 3 wk, and subsequently 1300 mg kg⁻¹ diet.

The dose was the maximum tolerated for young mice, but not necessarily for adults. At 78 wk of age 65/72 mice were still alive. There was no significant difference in the incidence of tumours between treated and control animals (20).

Oral mouse (3 month) 3500 mg kg⁻¹ wk⁻¹ for 6 wk. 41/180 developed lung adenomas compared with 30/184 controls (21).

Gavage rat (22 month) 285 mg kg⁻¹ 2 × wk⁻¹ for life. 10/60 survived at 22 month, of which 2 had tumours (1 adenocarcinoma and 1 lymphosarcoma of the intestine). 1/46 controls still alive at 22 months developed a fibrosarcoma (22).

Subcutaneous rat (22 month) 20 mg kg⁻¹ implant in paraffin. Of 6/48 rats which survived for 20 months, 4 developed tumours (1 malignant hepatoma, 1 fibrosarcoma, 1 spindle-cell sarcoma and 1 rhabdomyosarcoma). 1/46 controls which survived 22 months developed a fibrosarcoma (22).

Subcutaneous mouse (17 month) single injection of 1000 mg kg⁻¹ on day 28 of life. 69/72 mice were still alive at wk 78 of age. 5/36 ♂ mice developed systemic reticulum-cell sarcomas, compared with 8/141 controls. There was no other increase in tumour incidence over that in controls (23).

Prenatal mouse, single intraperitoneal dose of 8 mg animal⁻¹ during the second half of pregnancy, 11/18 pregnant mice produced a total of 38 offspring. 6/20 which survived 4 months developed lung adenomas compared with 0/20 in controls (24).

Teratogenicity and reproductive effects

Oral rat 100 mg kg⁻¹ day⁻¹ for ≤6 months caused retardation of first pregnancies and an increase in the incidence of sterility and foetal resorption. The offspring had crooked tails and reduced weight gain (25).

Oral rat, 2-8 g kg⁻¹ on day 11 or 13 of gestation resulted in congenital abnormalities in the foetuses. No adverse effect was observed at doses of 1 g kg⁻¹ day⁻¹ on days 2-21 of gestation, or when the rats were exposed by inhalation to 100 mg m⁻³ for 4 hr day⁻¹ from day 4 of gestation (26).

Gavage mouse, 2000 mg kg⁻¹ day⁻¹ on days 8-12 of gestation caused no teratogenic effects (27).

Metabolism and toxicokinetics

~20% of administered zineb was metabolised to ethylene thiourea, a known mutagen, teratogen and carcinogen, following oral administration to the rat and marmoset. Carbon disulfide and carbon dioxide were eliminated in exhaled air (28,29).

Sensitisation

Positive results recorded in patch tests carried out on agricultural workers (30).

Genotoxicity

Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537, with and without metabolic activation negative (31,32).

Escherichia coli WP2 *uvrA* reverse mutation with and without metabolic activation negative (32).

Escherichia coli *polA* primary DNA damage negative (32).

Drosophila melanogaster sex-linked recessive lethal assay positive (33).

In vitro human lung fibroblasts, unscheduled DNA synthesis negative (32).

Did not increase the frequency of somatic mutations in a heterozygous chlorophyll mutant of *Nicotiana tabacum* variant *xanthi* (34).

Other effects

Other adverse effects (human)

Workers exposed for ≤6 yr showed functional changes in the cardiovascular system which preceded clinically manifested pathological changes. An increase in the rate of occult bronchospasms caused by various respiratory effects was also reported (35).

One person suffering from hypocalasaemia developed sulphaemaglobinaemia, haemolytic anaemia and Heinz body formation after contact with zineb (36).

An increase in the number of chromosomal aberrations in peripheral blood lymphocytes was observed in a study of exposed workers (37).

Thyroid peroxidase (TPO) is thought to be the target for the thyroid toxicity of zineb. 5 µM inhibited TPO peroxidative activity in Chinese hamster ovary cells transfected with the human TPO gene. Iodination activity was blocked by 50 µM zineb. Inhibition of peroxidative activity was irreversible in the absence of iodine (38).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (39).

Pesticides and organometallic compounds are included in Schedule 6 (Release into Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (40).

WHO Toxicity Class Table 5 (41).

EPA Toxicity Class IV (formulation) (5).

ADI (JMPR) 0.03 mg kg⁻¹ body weight (5).

Other comments

Residues have been isolated from soils and on crops (42).

Environmental fate reviewed (42).

Residues on vegetables degrade to ethylenethiourea during cooking (1).

Uses, occurrence, analysis, genotoxicity, carcinogenicity and mammalian toxicity reviewed (43,44).

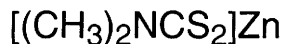
Autoignition temperature 149°C.

References

1. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
2. Tooby, E. E. et al *Chem. Ind. (London)* 21 June 1975.
3. van Leeuwen, C. J. et al *Aquat. Toxicol.* 1985, 7(3), 145-164.

4. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
5. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
6. Freitz, D. et al *Chemosphere* 1985, **14**, 1589-1616.
7. Haushik, M. et al *Int. J. Trop. Agric.* 1987, **5**(3-4), 190-198.
8. Rajagopal, B. S. et al *Residue Rev.* 1984, **93**, 1-199.
9. *Crop Protection Chemicals Reference* 2nd ed., 1986, 701-703, John Wiley, New York, NY, USA.
10. Nash, R. G. et al *J. Agric. Food Chem.* 1980, **28**, 322-330.
11. Konyk, L. V. et al *Khim. Tekhnol. Vody* 1987, **9**(2), 145-147 (Russ.) (*Chem. Abstr.* **107**, 12549b).
12. Kenaga, E. E. *Ecotoxicol. Environ. Saf.* 1980, **4**, 26-38.
13. Schafer, E. W. *Toxicol. Appl. Pharmacol.* 1972, **21**, 315-330.
14. *Gig. Sanit.* 1966, **31**(10), 25.
15. *J. Toxicol. Environ. Health* 1978, **4**, 93.
16. Izmerov, N. F. et al *Toxicometric Parameters of Industrial Toxic Chemicals Under Single Exposure* 1982, 121, CIP, Moscow, USSR.
17. Kaloyanova, F. et al *J. Hyg., Epidemiol., Microbiol., Immunol.* 1989, **33**(1), 11-17.
18. *IARC Monograph* 1987, **Suppl. 7**, 74.
19. Blackwell-Smith, et al *J. Pharmacol. Exp. Ther.* 1953, **109**, 159-166.
20. Innes, J. R. M. et al *J. Natl. Cancer Inst.* 1969, **42**, 1101-1114.
21. Chernov, O. V. et al *Vopr. Onkol.* 1969, **15**, 71-74.
22. Andrianova, M. M. et al *Vopr. Pitan.* 1970, **29**, 71-74.
23. *NTIS Evaluation of Carcinogenic, Teratogenic and Mutagenic Activities of Selected Pesticides and Industrial Chemicals* 1968, **1** (Carcinogenic Study), Dept. Commerce, Washington, DC, USA.
24. Kuitnitskaya, V. A. et al *Vopr. Pitan.* 1971, **30**, 49-50.
25. Ryazanova, R. A. *Gig. Sanit.* 1967, **32**, 26-30.
26. Petrova-Vergieva, T. et al *Food Cosmet. Toxicol.* 1973, **11**, 239-244.
27. Kavlock, R. J. et al *Teratog., Carcinog., Mutagen.* 1987, **7**(1), 7-16.
28. Searle, A. et al *Xenobiotica* 1987, **17**(6), 733-740.
29. Truhaut, R. et al *C. R. Acad. Sci., (Ser. 3)* 1973, **276**, 229-233.
30. Lisi, P. et al *Contact Dermatitis* 1986, **15**(5), 266-269.
31. Zeiger, E. et al *Environ. Mol. Mutagen.* 1988, **11**(Suppl. 12), 1-158.
32. Garrett, N. E. et al *Mutat. Res.* 1986, **168**(3), 301-325.
33. Tripathy, N. K. et al *Mutat. Res.* 1988, **206**(1), 25-31.
34. Briza, J. *Biol. Plant.* 1989, **31**(2), 145-151.
35. Kolpikov, I. E. et al *Gig. Tr. Prof. Zabol.* 1987, **(6)**, 35-38 (Russ.) (*Chem. Abstr.* **107**, 182617q).
36. Pinkhas, J. et al *Blood* 1963, **21**, 484-494.
37. Pilinskaya, M. A. *Genetika (Moscow)* 1974, **10**, 140-146.
38. Marinovich, M. et al *Arch. Toxicol.* 1997, **71**(8), 508-512.
39. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
40. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
41. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
42. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1991, **3**, 657-662, Lewis Publishers, Chelsea, MI, USA.
43. *IARC Monograph* 1976, **12**, 245-257.
44. Franekic, J. et al *Comparative Genetic Toxicity of Some Pesticides. Chemical Safety International Reference Manual* 1994, 141-156, Richardson, M. L. (Ed.), VCH Publishers, Weinheim, Germany

Z19 ziram



$\text{C}_6\text{H}_{12}\text{N}_2\text{S}_4\text{Zn}$

Mol. Wt. 305.83

CAS Registry No. 137-30-4

Synonyms Attivar; Carbazinc; Corozate; Cuman; Fungizir; Mezene; Pomarsol Z; Triscabol; methyl zimate; (*T*₄)-bis(dimethyldithiocarbamate-*S,S'*)zinc; zinc bis(dimethyldithiocarbamate); zinc *N,N*-dimethyldithiocarbamate

EINECS No. 205-288-3

RTECS No. ZH 0525000

Uses Fungicide. Wildlife repellent. Vulcanisation accelerator.

Physical properties

M. Pt. 246°C, 240-244°C (technical) **Specific gravity** 1.65 at 20°C with respect to water at 20°C

Partition coefficient log *P*_{ow} 1.086 (1)

Solubility Water: 0.03 mg l⁻¹ at 20°C. Organic solvents: soluble in benzene, chloroform, carbon disulfide, carbon tetrachloride; moderately soluble in acetone, naphtha

Occupational exposure

SE-LEVL 1 mg m⁻³

SE-STEL 2 mg m⁻³

Supply classification harmful

Risk phrases Harmful if swallowed – Irritating to eyes, respiratory system and skin – Possible risk of irreversible effects (R22, R36/37/38, R40)

Safety phrases Keep out of reach of children (if sold to general public) – Wear suitable protective clothing and gloves (S2, S36/37)

Ecotoxicity

Fish toxicity

LC₅₀ (5 hr) goldfish 5-10 mg l⁻¹ (2).

LC₅₀ (60 day) rainbow trout 2.0 µg l⁻¹ (3).

Invertebrate toxicity

EC₅₀ (15 min) *Photobacterium phosphoreum* 0.14 ppm Microtox test (4).

LC₅₀ (21 day) *Daphnia magna* 11 µg l⁻¹ (5).

Not toxic to bees. LD₅₀ >100 µg bee⁻¹ (6).

Bioaccumulation

Estimated bioconcentration factor 59 indicates that environmental accumulation is unlikely (7).

Environmental fate

Degradation studies

Ziram ionises to form dimethyldithiocarbamate ions that biodegrade in soil, releasing carbon disulfide and forming dimethylamine (8).

Biodegradation may be hindered through ziram's antibacterial properties, particularly towards Gram-positive bacteria (9).

Abiotic removal

Decomposed by UV radiation (2).

Adsorption and retention

Estimated *K*_{oc} 440 indicates moderate adsorption to soil (7).

Mammalian & avian toxicity

Acute data

LD₅₀ oral redwing blackbird 100 mg kg⁻¹ (10).

LD₅₀ oral rat 1400 mg kg⁻¹ (11).

LD₅₀ dermal rat >6000 mg kg⁻¹ (2).

LD₅₀ intraperitoneal rat, rabbit, guinea pig, mouse 5-23 mg kg⁻¹ (2,12).

Sub-acute and sub-chronic data

Oral ♂ rat, 5 or 25 mg kg⁻¹ day⁻¹ for 30, 60 or 90 days caused significant mortality. An increased thyroid:body weight ratio and reduced thyroid iodine uptake and protein-bound iodine were also reported. However, no change in the clinical enzyme profile of the liver, serum and brain were noted. It is believed that the metabolite ethylene thiourea was responsible for the high mortality and effects on the thyroid (13).

Carcinogenicity and chronic effects

No adequate evidence for carcinogenicity to humans, insufficient evidence for carcinogenicity to animals, IARC classification group 3 (14).

Oral rat, 5 mg kg⁻¹ day⁻¹ for 1 yr caused no adverse effects (2).

Gavage mouse, 4.6 mg kg⁻¹ day⁻¹ for 3 wk, then 15 mg kg⁻¹ diet for 74 wk. Tumour incidences were not significantly different from that in controls (15).

Gavage rat 70 mg kg⁻¹ 2 × wk⁻¹ for 22 months. Survival rates were 10/60 among treated and 46/60 in controls. Tumour incidences were 2 malignant hepatomas and 2 fibrosarcomas in treated rats, and 1 fibrosarcoma among controls (16).

Subcutaneous implant (22 month) 15 mg in 250 mg paraffin pellet. Among 10/48 survivors, 3 developed tumours (1 hepatoma, 1 fibrosarcoma, 1 lymphosarcoma of the intestine). No tumours occurred at the sight of implantation. Of 46 controls, which did not receive paraffin pellets and were still alive at 22 months, 1 developed a fibrosarcoma (16).

Subcutaneous mouse (74 wk) single injection of 46.4 mg kg⁻¹. Survival rates were 13/18 to 17/18 among 4 groups of 2 strains both sexes. Tumour incidences were not significantly different from control groups (17).

Oral rat 0, 20, 200 or 2000 ppm diet for 2 yr. Epiphyseal abnormalities in the long bones of the hind legs were observed in rats fed the high dose. 3/80 high does ♂ rats also showed partial paralysis of the hind limbs (18).

Teratogenicity and reproductive effects

Gavage ♀ rats on gestation days 1-5 (preimplantation study 0, 25, 50 and 100 mg kg⁻¹) or during organogenetic period (teratogenic study 0, 12.5, 25, 50 and 100 mg kg⁻¹). Study was terminated on day 21 of gestation. In the preimplantation study foetal weights were reduced in animals treated with 50 and 100 mg kg⁻¹. In the teratogenic study a slight dismorphogenic effect was observed in animals treated with 50 and 100 mg kg⁻¹. Embryofoetotoxic effects appeared when exposure concentrations ≥25 mg kg⁻¹. Maternal toxicity was evident at all doses (19).

Administration to mice of 50 mg kg⁻¹ day⁻¹ for 15 days reduced the fertility and fecundity of ♀, but did not affect the fertility of ♂ mice (ratio unspecified) (20).

Metabolism and toxicokinetics

Water-soluble metabolites were found in the blood, kidneys, liver, ovaries, spleen and thyroid of ♀ rats 24 hr after oral administration. Unchanged ziram was found in the faeces. The presence of water-soluble metabolites indicates the generation of the dimethyldithiocarbamate ion in the stomach after ingestion (21,22).

Irritancy

Irritating to the skin and mucous membranes (species unspecified) (2).

Sensitisation

Skin patch tests were carried out in 348 subjects, irritation was recorded in agricultural workers, but not in ex-agricultural workers (23).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA1535 with metabolic activation positive (24).

Bacillus subtilis H17, M45 rec-assay positive (25).

Drosophila melanogaster sex-linked recessive lethal assay positive, induction of translocations negative (26).
In vitro mouse lymphoma L5178Y cells, tk⁺/tk⁻ forward mutation positive (27).
In vitro Chinese hamster ovary cells, sister chromatid exchanges negative, chromosomal aberrations positive (28).
In vivo mouse bone marrow cells, chromosomal aberrations positive (29).
In vivo ♂ mouse bone marrow cells, induction of micronuclei positive, ♂ mouse germ cells, chromosomal aberrations positive (30).

Other effects

Other adverse effects (human)

Thyroid peroxidase (TPO) is thought to be the target for the thyroid toxicity of ziram. 5 µM ziram inhibited TPO peroxidative activity in Chinese hamster ovary cells transfected with the human TPO gene (31).

Any other adverse effects

Intraperitoneal rat, single injection of 10 mg kg⁻¹ elicited a glycogenolytic response (32).

Like most dithiocarbamates, ziram induces the accumulation of acetaldehyde in the blood of rats simultaneously administered ethanol (33).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Pesticides: maximum admissible concentration 0.1 µg l⁻¹ (34).

Included in Schedule 6 (Release into the Land: Prescribed Substances) Statutory Instrument No. 472, 1991 (35).

WHO Toxicity Class III (36).

EPA Toxicity Class III (formulation) (6).

ADI (JMPR) 0.02 mg kg⁻¹ body weight (6).

Other comments

Only very low levels have been detected on crops (37).

Environmental fate reviewed (37).

Physical properties, uses, analysis, genotoxicity, carcinogenicity and mammalian toxicity reviewed (23,38,39).

References

1. McCoy, G. D. et al *Carcinogenesis* 1990, **11**(7), 1111-1117.
2. *The Agrochemicals Handbook* 3rd ed., 1991, The Royal Society of Chemistry, London, UK.
3. van Leeuwen, C. J. et al *Aquat. Toxicol.* 1986, **9**(2-3), 129-145.
4. Kaiser, K. L. E. et al *Water Pollut. Res. J. Can.* 1991, **26**(3), 361-431.
5. van Leeuwen, C. J. et al *Aquat. Toxicol.* 1985, **7**(3), 165-175.
6. *The Pesticide Manual* 11th ed., 1997, The British Crop Protection Council, Farnham, UK.
7. Kenaga, E. E. *Ecotoxicol. Environ. Saf.* 1980, **4**, 26-38.
8. Rajagopal, B. S. et al *Residue Rev.* 1984, **93**, 1-199.
9. Hansen, J. C. *Chemosphere* 1972, **1**, 159-162.
10. Schafer, E. W. *Toxicol. Appl. Pharmacol.* 1972, **21**, 315-330.
11. *Farm Chemicals Handbook* 1980, C259, Meister Publ., Willoughby, OH, USA.
12. *Environ. Qual. Saf.* 1975, **3**, 618.
13. Pandey, M. et al *Environ. Pollut.* 1990, **65**(4), 311-322.
14. Dailey, R. E. et al *J. Agric. Food Chem.* 1969, **17**, 827-828.
15. *IARC Monograph* 1987, **Suppl. 7**, 74.
16. Innes, J. R. M. et al *J. Natl. Cancer Inst.* 1969, **42**, 1101-1114.
17. Andrianova, M. M. et al *Vap. Pitan.* 1970, **29**, 71-74.
18. *NTIS Evaluation of Carcinogenic, Teratogenic and Mutagenic Activities of Selected Pesticides and Industrial Chemicals* 1968, 1(Carcinogenic Study), US Dept. Commerce, Washington, DC, USA.
19. Enomoto, A. et al *Toxicology* 1989, **54**(1), 45-58.
20. *Ecotoxicol. Environ. Saf.* 1983, **7**, 531.
21. Ghezzer, F. et al *Quad. Sclavo. Diagn.* 1972, **8**, 485-494.

22. Izmirov, N. et al *Eksp. Med. Morfol.* 1972, **11**, 152-156.
23. *IARC Monograph* 1976, **12**, 259-270.
24. Lisi, P. et al *Contact Dermatitis* 1987, **17**, 212-218.
25. Zeiger, E. *Cancer Res.* 1987, **47**, 1287-1296.
26. Shimasu, Y. et al *Mutat. Res.* 1976, **40**, 19-30.
27. Hemavathy, K. C. et al *Environ. Mol. Mutagen.* 1989, **14**(4), 252-253.
28. McGregor, D. B. et al *Environ. Mol. Mutagen.* 1988, **12**(1), 85-154.
29. Gulati, D. K. et al *Environ. Mol. Mutagen.* 1989, **13**(2), 133-193.
30. Antonovich, E. A. *Proc. Symp. Toxicol. Anal. Chem. Diethiocarbamates, Dubrovnic* 1970, 3-20.
31. Marinovich, M. et al *Arch. Toxicol.* 1997, **71**(8), 508-512.
32. Hemavathy, K. C. et al *Mutat. Res.* 1988, **208**(1), 57-60.
33. van Lagten, M. J. *Diethiocarbamat Alcohol Reactive bij de Rat* 1972, 40, Bedrijf FA Jammers, Terhorg, Netherlands.
34. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
35. *S. I. 1991 No. 472 The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
36. *The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification* 1998-1999 WHO/PCS/98.21.
37. Howard, P. H. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* 1991, **3**, 663-667, Lewis Publ., Chelsea, MI, USA.
38. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium.
39. Franekic, J. et al *Comparative Genetic Toxicity of Some Pesticides. Chemical Safety International Reference Manual* 1994, 141-156, Richardson, M. L. (Ed.), VCH Publishers, Weinheim, Germany

20 zirconium

Zr

Zr

Mol. Wt. 91.22

CAS Registry No. 7440-67-7

EINECS No. 231-176-9

RTECS No. ZH 7070000

Uses In deodorants. In atomic reactors. In explosives. In lamp filaments.

Occurrence In minerals, zircon, malacon, baddeleyite, zirkelite, eudialyte. Frequently found in rare-earth minerals and in monazite sand. Constitutes 0.023 % of Earth's crust.

Physical properties

M. Pt. 1857°C B. Pt. 3577°C Specific gravity 6.500

Occupational exposure

DE-MAK 1 mg m⁻³ (inhalable fraction of aerosol)

US-TWA 5 mg m⁻³

US-STEL 10 mg m⁻³

UN No. 2008 (dry powder)

UN No. 1358 (wetted powder)

UN No. 2009 (dry finished sheets, strip or coiled wire)

UN No. 2858 (dry coiled wire, finished metal sheets thinner than 254 microns but not thinner than 18 microns)

HAZCHEM Code 4Y (dry powder) **HAZCHEM Code** 1Z (wetted powder) **HAZCHEM Code** 4Z (dry coiled wire, finished metal sheets thinner than 254 microns but not thinner than 18 microns) **Conveyance classification** spontaneously combustible substance (dry powder and dry finished sheets, strip or coiled wire) **Conveyance classification** flammable solid (wetted powder and dry coiled wire, finished metal sheets thinner than 254 microns but not thinner than 18 microns)

Supply classification highly flammable (zirconium powder pyrophoric)

Risk phrases zirconium powder non-pyrophoric – Contact with water liberates extremely flammable gases – zirconium powder pyrophoric - Contact with water liberates extremely flammable gases – Spontaneously flammable in air (R15, R15, R17)

Safety phrases Keep out of reach of children (if sold to general public) – Keep container tightly closed and dry – In case of fire, use class D extinguisher – never use water or carbon dioxide (S2, S7/8, S43)

Ecotoxicity

Fish toxicity

LC₅₀ (96 hr) fish (unspecified) bioassay >20 mg l⁻¹ (1).

Invertebrate toxicity

EC₅₀ (5 min) *Photobacterium phosphoreum* >4.3 mg l⁻¹ Microtox test (1).

Mammalian & avian toxicity

Sub-acute and sub-chronic data

Intraperitoneal mouse, doses of zirconium oxychloride at 1/200 or 1/400 LD₅₀ every other day for 2, 4 or 6 months, and single doses of zirconium oxychloride, zirconium oxide and zirconium silicate at 1/10 or 1/100 LD₅₀ into the thorax cavity, enhanced the level of IgM plaque-forming cells against sheep red blood cells in the spleen of mice (2).

Sensitisation

Many individuals exposed to zirconium and its salts develop cell (T-lymphocyte)-mediated delayed skin hypersensitivity, followed by the appearance of immunological granulomas (3).

Genotoxicity

Escherichia coli SOS-Chromotest negative (1).

Salmonella typhimurium TA98, TA100, TA102, TA1537, TA2637 negative. When tested in combination with 9-aminoacridine, the mutation rate was higher than that for 9-aminoacridine alone (zirconium tetrachloride) (4).

Other effects

Other adverse effects (human)

Granulomatous lesions, probably of allergic epithelioid origin, have been observed following the use of deodorant sticks and poison ivy lotions containing zirconium (form unspecified) (5).

Chest radiographs were taken in 1975, 1978 and 1982 and lung function measurements for 1975 to 1988 obtained for 178 men with extended exposure to zirconium compounds at concentrations mainly <10 mg m⁻³. An estimate of cumulative exposure was derived from job title and probable exposure in each work area. No evidence that exposure to zirconium compounds results in abnormal chest radiographs or impaired pulmonary function was found (6).

Legislation

Included in Schedule 4 (Release into Air: Prescribed Substances) Statutory Instrument No. 472, 1991 (7).

Other comments

Reviews on human health effects, experimental toxicology, physico-chemical properties listed (8).

References

1. Coutive, P. et al *Water, Air, Soil Pollut.* 1989, **47**(1-2), 87-100.
2. Nagaoka, K. et al *Rodo Kagaku* 1988, **64**(1), 27-33 (Japan.) (*Chem. Abstr.* **108**, 181780w).
3. Price, R. J. et al *Toxicol. Lett.* 1986, **30**, 89-95.
4. Iyehara, O. et al *Jpn. J. Genet.* 1987, **62**(2), 159-162.

5. Doull, J. et al (Eds.) *Casarett and Doull's Toxicology* 2nd ed., 1980, 462, MacMillan, New York, NY, USA.
6. Marcus, R. L. et al *Occup. Med.* 1996, **46**(2), 109-113.
7. S. I. 1991 No. 472 *The Environmental Protection (Prescribed Processes and Substances) Regulations* 1991, HMSO, London, UK.
8. *ECETOC Technical Report No. 71* 1996, European Centre for Ecotoxicology and Toxicology of Chemicals, 4 Avenue E. Van Nieuwenhuyse (Bte 6), B-1160 Brussels, Belgium

221 zirconium hydride



H_2Zr

Mol. Wt. 93.24

CAS Registry No. 7704-99-6

Synonyms zirconium dihydride

EINECS No. 231-727-3

RTECS No. ZH 8015000

Uses Catalyst. In nuclear reactor fuel assemblies. Powerful reducing agent at high temperatures. Self-igniter in propellants and pyrotechnics.

Occupational exposure

DE-MAK 1 mg m⁻³ (inhalable fraction of aerosol)

UK-LTEL 5 mg m⁻³ (as Zr)

UK-STEL 10 mg m⁻³ (as Zr)

US-TWA 5 mg m⁻³ (as Zr)

US-STEL 10 mg m⁻³ (as Zr)

UN No. 1437 HAZCHEM Code 2Z Conveyance classification flammable solid

Mammalian & avian toxicity

Irritancy

Irritating to the skin, eyes, mucous membranes and upper respiratory tract (species unspecified) (1).

Other effects

Other adverse effects (human)

Manufacture has been associated with incidence of pulmonary granuloma (2).

Other comments

Autoignition temperature 132°C.

References

1. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, 2, 3634, Sigma-Aldrich, Milwaukee, WI, USA.
2. Shkurko, G. A. *Gig. Tr.* 1973, 9, 74-76 (Russ.) (*Chem. Abstr.* 85, 129779v)

222 zirconium nitrate



$\text{N}_4\text{O}_{12}\text{Zr}$

Mol. Wt. 339.24

CAS Registry No. 13746-89-9

Synonyms zirconium tetranitrate

EINECS No. 237-324-9

RTECS No. ZH 8750000

Uses Catalyst.

Physical properties

M. Pt. 100°C (decomp.)

Solubility Water: very soluble. Organic solvents: ethanol

Occupational exposure

DE-MAK 1 mg m⁻³ (inhalable fraction of aerosol)

UK-LTEL 5 mg m⁻³ (as Zr)

UK-STEEL 10 mg m⁻³ (as Zr)

US-TWA 5 mg m⁻³ (as Zr)

US-STEEL 10 mg m⁻³ (as Zr)

UN No. 2728 HAZCHEM Code 1Y Conveyance classification oxidising substance

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 2300 mg kg⁻¹ (1).

LC_{Lo} (30 min) inhalation rat 500 mg m⁻³ (2).

Genotoxicity

Salmonella typhimurium TA1535/psk1002 Ames test negative (3).

Other effects

Other adverse effects (human)

Extremely destructive to tissues of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema (4).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Nitrates: guide level 25 mg l⁻¹, maximum admissible concentration 50 mg l⁻¹ (5).

References

1. Lewis, R. J. (Ed.) *Sax's Dangerous Properties of Industrial Materials* 8th ed., 1992, Van Nostrand Reinhold, New York, NY, USA.
2. *NTIS Report AEC-TR6710* Natl. Tech. Inf. Ser., Springfield, VA, USA.
3. Nakamura, S. et al *Sangyu Igaka* 1989, **31**(6), 430-431.
4. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3636, Sigma-Aldrich, Milwaukee, WI, USA.
5. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

223 zirconium(IV) sulfate



$\text{O}_8\text{S}_2\text{Zr}$

Mol. Wt. 283.35

CAS Registry No. 14644-61-2

Synonyms disulfatozirconic acid; sulfuric acid, zirconium(IV) salt (2:1); zircenyl sulfate; zirconium sulfate

EINECS No. 238-694-4

RTECS No. ZH 9100000

Uses Catalyst. Tanning of leather.

Physical properties

M. Pt. 410°C (decomp.) **Specific gravity** 3.22 at 16°C

Solubility Water: 525 g l⁻¹ at 18°C. Organic solvents: ethanol

Occupational exposure

DE-MAK 5 mg m⁻³ (as Zr) (inhalable dust fraction)

UK-LTEL 5 mg m⁻³ (as Zr)

UK-STEL 10 mg m⁻³ (as Zr)

US-TWA 5 mg m⁻³ (as Zr)

US-STEL 10 mg m⁻³ (as Zr)

Mammalian & avian toxicity

Acute data

LD₅₀ oral rat 3500 mg kg⁻¹ (1).

LD₅₀ intraperitoneal rat 175 mg kg⁻¹ (1).

LD_{Lo} subcutaneous rat 500 mg kg⁻¹ (2).

Teratogenicity and reproductive effects

Intratesticular ♂ rat, lowest toxic dose 23 mg kg⁻¹ 1 day prior to mating, parameters studied: effects on testes, epididymis and sperm duct (3).

Irritancy

Irritating to the eyes, skin, mucous membranes and upper respiratory tract (species unspecified) (4).

Other effects

Any other adverse effects

In vitro mouse splenocytes, mitogenic effect was demonstrated by a concentration-dependent stimulation of cell proliferation, as measured by an increase in tritiated thymidine incorporation into lymphocyte DNA (5).

Legislation

Limited under EC Directive on Drinking Water Quality 80/778/EEC. Sulfates: guide level 25 mg l⁻¹, maximum admissible concentration 250 mg l⁻¹ (6).

References

1. Cochran, et al *Arch. Ind. Hyg. Occup. Med.* 1950, 1, 637.
2. NTIS Report AEC-TR-6710 Natl. Tech. Inf. Ser., Springfield, VA, USA.
3. *J. Repro. Fertil.* 1964, 7, 21.
4. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, 2, 3634, Sigma-Aldrich, Milwaukee, WI, USA.
5. Price, R. J. et al *Toxicol. Lett.* 1986, 30, 89-95.
6. EC Directive Relating to the Quality of Water Intended for Human Consumption 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg

224 zirconium tetrachloride



Cl_4Zr

Mol. Wt. 233.03

CAS Registry No. 10026-11-6

Synonyms zirconium chloride; zirconium(IV) chloride

EINECS No. 233-058-2

RTECS No. ZH 7175000

Uses Catalyst. Chemical synthesis. Electrolyte.

Physical properties

M. Pt. 331°C (subl.) B. Pt. 437°C Specific gravity 2.803 at 15°C Volatility v.p. 1 mmHg at 190°C

Solubility Water: decomposed by water to form ZrOCl_2 and HCl. Organic solvents: diethyl ether, ethanol

Occupational exposure

DE-MAK 1 mg m⁻³ (inhalable fraction of aerosol)

UK-LTEL 5 mg m⁻³ (as Zr)

UK-STEL 10 mg m⁻³ (as Zr)

US-TWA 5 mg m⁻³ (as Zr)

US-STEL 10 mg m⁻³ (as Zr)

UN No. 2503 HAZCHEM Code 4WE Conveyance classification corrosive substance

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, rat 490, 1700 mg kg⁻¹, respectively (1,2).

Genotoxicity

Salmonella typhimurium TA98, TA100, TA102, TA1537, TA2637 negative. When tested in combination with 9-aminoacridine, the mutation rate was higher than for 9-aminoacridine alone (3).

Other effects

Other adverse effects (human)

Extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and oedema of the larynx and bronchi, chemical pneumonitis and pulmonary oedema (4).

Legislation

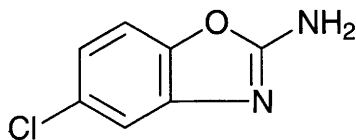
Limited under EC Directive on Drinking Water Quality 80/778/EEC. Chlorides: guide level 25 mg l⁻¹ (5).

UK maximum admissible concentration in drinking water, chloride 400 mg l⁻¹ (12-monthly average) (6).

References

1. *J. Pharmacol.* 1983, **14**, 437.
2. *Hyg. Sanit.* 1966, **31**, 328.
3. Iychara, O. et al *Jpn. J. Genet.* 1987, **62**(2), 159-162.
4. Lenga, R. E. *Sigma-Aldrich Library of Chemical Safety Data* 2nd ed., 1988, **2**, 3634, Sigma-Aldrich, Milwaukee, WI, USA.
5. *EC Directive Relating to the Quality of Water Intended for Human Consumption* 1982, 80/778/EEC, Office for Official Publications of the European Communities, 2 rue Mercier, L-2985 Luxembourg.
6. *S.I. 1991 No. 1147, The Water Supply (Water Quality) Regulations 1991*, HMSO, London, UK

225 zoxazolamine



C₇H₅ClN₂O

Mol. Wt. 168.58

CAS Registry No. 61-80-3

Synonyms 2-amino-5-chlorobenzoxazole; 5-chloro-2-benzoxazolamine; Deflexol; Flexilon; MCN-485; zoxamin

EINECS No. 200-519-4

RTECS No. DM 4550000

Uses Skeletal muscle relaxant. Uricosuric.

Physical properties

M. Pt. 184-185°C

Solubility Organic solvents: methanol, propylene glycol

Mammalian & avian toxicity

Acute data

LD₅₀ oral mouse, hamster, rat 540, 670, 780 mg kg⁻¹, respectively (1-3).

LD₅₀ intraperitoneal mouse, rat, hamster 100, 102, 270 mg kg⁻¹, respectively (3,4).

LD₅₀ intravenous mouse, dog 120, 380 mg kg⁻¹, respectively (1,5).

Other effects

Other adverse effects (human)

Oral human, lowest toxic dose 14 mg kg⁻¹, central nervous system effects (6).

Other comments

Metabolites had no significant pharmacological effect in rats (5).

References

1. *Arch. Int. Pharmacodyn. Therap.* 1960, **128**, 112.
2. *J. Pharmacol. Exp. Ther.* 1960, **129**, 75.
3. *Fed. Am. Soc. Exp. Biol. Proc.* 1957, **16**, 319.
4. *NTIS Report AD277-689* Natl. Tech. Inf. Ser., Springfield, VA, USA.
5. Yasuhara, M. et al *Pharm. Res.* 1988, **5**(7), 401-407.
6. *J. Am. Med. Assoc.* 1956, **160**, 745

Indexes

Index of Chemical Names and Synonyms

- 0-2857 **B76**
 666 **H10**
 A100 **I70**
 A150 **V39**
 A306 **S132**
 A 4766 **D371**
 A 5089 **D371**
 Aadimethoat **D376**
 AAF **A23**
 Aarane **S57**
 Aaroson **D593**
 AAservo **C312**
 AAterra **E185**
 Aatrex **A252**
 Abate **T19**
 Abathion **T19**
 Abbaflor **F41**
 Abbalide **G2**
 Abbotcin **E47**
 Abboxide **C120**
 7,13-abietadien-18-oic acid **A2**
 abietic acid **A2**
 (–)-abietic acid **A2**
 ABL **L8**
 Ablumide DEA **L7**
 Ablusol DBC **C32**
 Abluton T30 **C163**
 Abol X **M50**
 Abricycline **T62**
 absolute alcohol **E61**
 Abstensil **D565**
 AC-92,100 **T22**
 A- α -C **A1**
 AC222293 **I5**
 AC243997 **I6**
 AC263,499 **I7**
 AC 47470 **M56**
 AC 92553 **P20**
 Acaflor **H80**
 Acamichem **D504**
 Acanal **B187**
 Acanor **F7**
 Acaphid **D566**
 Acaralate **C276**
 Acarcide **T63**
 Acared **D261**
 Acarelte **D504**
 Acarfen **D261**
 Acaril **B187**
 Acarion **P300**
 Acaristop **C357**
 Acarmate **B81**
 Acaroil TD **T63**
 Acarol **B187**
 Acarox **C535**
 Acarpec **C535**
 Acarstin **C535**
 Accelerate **E22**
 Acclaim **F16**
 Acconem **F109**
 Accothion **F11**
 Accutane **I138**
 Acemeco **M40**
 acenaphthene **A3**
 acenaphthylene **A4**
 acephate **A5**
 Aceptate-met **M111**
 acetal **A6**
 acetaldehyde **A7**
 acetaldehyde diethyl acetal **A6**
 acetaldehyde dimethyl acetal **D380**
 acetaldehyde formylmethylhydrazone **A8**
 acetaldehyde *N*-methyl-*N*-formylhydrazone **A8**
 acetaldehyde oxime **A9**
 acetaldehyde tetramer **M94**
 acetaldol **A63**
 acetaldoxime **A9**
 acetamide **A10**
 acetamide, *N*-(aminothiooxomethyl) **A29**
 acetamide, *N*-(butoxymethyl)-2-chloro-*N*-(2,6-diethyl-phenyl)-*N*-butoxymethyl-2-chloro-2',6'-diethylacetanilide **B196**
 acetamide, *N*-[4-(chloroacetyl)phenyl]- **C150**
 acetamide, 2-cyano-*N*-[(ethylamino)carbonyl]-2-(methoxyimino)- **C541**
 acetamide, *N*-(1-cyano-1-methylethyl)-2-mercapto-, *S*-ester with *O,O*-diethyl phosphorothioate **C490**
 acetamide, 2-(diethylamino)-*N*-(2,6-dimethylphenyl)- **L43**
 acetamide, *N*-(4-((2-hydroxy-5-methylphenyl)azo)phenyl)- **C410**
 4-acetamidobiphenyl **P90**
 7-acetamido-6,7-dihydro-1,2,3,10-tetramethoxybenzo[*a*]heptalen-9(5,5*H*)one **C384**
 2-acetamidofluorene **A23**
 2-acetamido-5-nitrothiazole **A31**
p-acetamidophenacyl chloride **C150**
p-acetamidophenol **P6**
 4-(acetamido)phenyl 2-acetoxybenzoate **B33**
 4-acetamidophenylacetylsalicylate **B33**
 Acetamine Yellow CG **C410**

2-acetaminofluorene **A23**
 acetaminophen **P6**
 acetanilide **A11**
 Acetate fast orange R **A130**
 acetate PA **A90**
 (acetato-O)methylmercury **M250**
 acetatotriphenylstannane **F25**
 (acetato)tris(arsenito)dicropper **C431**
 acetdimethylamide **D383**
 Ace-Thios **D376**
 acetic acid **A12**
 acetic acid, allyl ester **A72**
 acetic acid amide **A10**
 acetic acid, amyl ester **A195**
 acetic acid, anhydride **A13**
 acetic acid, barium salt **B6**
 acetic acid, benzyl ester **B88**
 acetic acid bromide **A24**
 acetic acid, bromo-, benzyl ester **B93**
 acetic acid, bromo-, 2-butene-1,4-diyl ester **B114**
 acetic acid, bromo-, phenylmethyl ester **B93**
 acetic acid, *sec*-butyl ester **B234**
 acetic acid, *tert*-butyl ester **B235**
 acetic acid, cadmium salt **C3**
 acetic acid chloride **A25**
 acetic acid, chromium(3+) salt **C332**
 acetic acid, copper(2+) salt **C430**
 acetic acid, dichloro- **D172**
 acetic acid, 1,3-dimethylbutyl ester **H77**
 acetic acid, 1,1-dimethylethyl ester **B235**
 acetic acid ethenyl ester **V26**
 acetic acid, isobutyl ester **I87**
 acetic acid, isopropenyl ester **I118**
 acetic acid, lead(IV) salt **L32**
 acetic acid, mercapto-, 2-ethylhexyl ester **E134**
 acetic acid, mercury(2+) salt **M65**
 acetic acid, 2-methyl-2-propene-1,1-diol diester **M104**
 acetic acid, 1-methylpropyl ester **B234**
 acetic acid, monoammonium salt **A162**
 acetic acid, 2-phenylethyl ester **P66**
 acetic acid, phenylmethyl ester **B88**
 acetic acid, 2-propenyl ester **A72**
 acetic acid, trichloro-, compound with *N'*-(4-chlorophenyl)-*N,N*-dimethylurea (1:1) **M351**
 acetic acid, (2,4,5-trichlorophenoxy)- **T1**
 acetic acid, trichlorosodium salt **S97**
 acetic acid vinyl ester **V26**
 acetic aldehyde **A7**
 acetic anhydride **A13**
 acetic bromide **A24**
 acetic chloride **A25**
 acetic ether **E87**
 acetic oxide **A13**
 acetic peroxide **P51**
 acetimidoylphosphoramidothioic acid, *O,O*-bis(*p*-chlorophenyl)ester **P148**
 acetoacetic acid butyl ester **B236**
 acetoacetic ester **E88**
 acetochlor **A14**
 acetocyanohydrin **L2**
 acetoferate **P215**
 acetohexamide **A15**
 acetomethoxane **D377**
 acetonanil **A16**
 acetone **A17**
 acetone cyanohydrin **A18**
 acetone glycerin ketal **S101**
 acetone ketal of glycerine **S101**
 acetone thiosemicarbazide **A19**
 acetonitrile **A20**
 acetonitrile, dibromo- **D122**
 acetonitrile, dichloro- **D175**
 acetonylacetone **H62**
 3-(α -acetonylbenzyl)-4-hydroxycoumarin **W1**
R-(+)-3-(α -acetonylbenzyl)-4-hydroxycoumarin **W2**
 3-(α -acetonylbenzyl)-4-hydroxycoumarin sodium salt **W3**
 acetonyl chloride **C146**
 3-(α -acetonyl-*p*-chlorobenzyl)-4-hydroxycoumarin **C445**
 3-(α -acetonylfurfuryl)-4-hydroxycoumarin **F116**
 acetonyl methyl ether **M131**
 Aceto PBN **P124**
p-acetophenetidine **P58**
 acetophenidin **P58**
 acetophenone **A21**
 Acetoquat CPC **C104**
 acetoquinone blue L **C409**
 acetoquinone light orange JL **A130**
 Acetosan **T50**
 Aceto SDD 40 **S64**
 acetothioamide **T115**
 2-acetoxybenzoic acid **A28**
 2-acetoxybutane **B234**
 17-acetoxy-6-chloro-6-dehydropregesterone **C139**
 acetoxyethane **E87**
 1-acetoxyethylene **V26**
 2-acetoxy-1-methoxypropane **M148**
 acetoxymethylmercury **M250**
 17 α -acetoxy-6-methylpregna-4,6-diene-3,20-dione **M44**
 2-acetoxypentane **P46**
 acetoxyphenylmercury **P116**
 2-acetoxypropene **I118**
 3-acetoxypropene **A72**
 α -acetoxytoluene **B88**
 acetylacetone **A22**
 acetyladiamycin **D23**
 acetylaminobenzene **A11**
 4-acetylaminobiphenyl **P90**
 2-acetylaminofluorene **A23**
N-acetyl-2-aminofluorene **A23**
 2-acetyl-amino-4-(5-nitro-2-furyl)thiazole **N117**
 4-acetyl-amino-2-nitrophenetole **N72**
 2-acetyl-amino-5-nitrothiazole **A31**
p-(acetyl-amino)phenacyl chloride **C150**
N-acetyl-*p*-aminophenol **P6**

(8*S*-*cis*)-8-acetyl-10-[(3-amino-2,3,6-trideoxy- α -L-*lyxo*-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-1-methoxy-5,12-naphthacenedione **D23**
 acetyl anhydride **A13**
 acetylaniline **A11**
 acetylbenzene **A21**
 1-(*p*-acetylbenzenesulfonyl)-3-cyclohexylurea **A15**
 acetyl benzoyl aconine **A33**
 acetyl bromide **A24**
 acetyl *tert*-butyl peroxide **B270**
 acetyl chloride **A25**
 acetyl chloride, dichloro- **D176**
cis-1-acetyl-4-[4-[[2-(2,4-dichlorophenyl)-2-(1*H*-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]-piperazine **K9**
 acetylen **A26**
 acetylene **A26**
 acetylene black **C73**
cis-acetylene dichloride **D213**
trans-acetylene dichloride **D214**
 acetylene, dichloro- **D177**
 acetylene tetrabromide **T40**
 acetylene tetrachloride **T50**
 acetyl enheptin **A31**
 acetylenogen **C24**
 acetyl ether **A13**
 acetylene **M318**
 acetylformic acid **P368**
 acetyl hydroperoxide **P51**
 3-acetyl-4-hydroxy-6-methyl-2*H*-pyran-2-one (enol form) **D45**
 acetyl iodide **A27**
 acetyl ketene **D363**
 acetyl mercaptan **T116**
N-acetyl-5-methoxytryptamine **M48**
 3-acetyl-6-methyl-2*H*-pyran-2,4(3*H*)-dione (keto form) **D45**
N-acetyl-1-naphthylamine **N21**
 4-acetylnitrobenzene **N73**
p-acetylnitrobenzene **N73**
 acetyl oxide **A13**
 2-acetyloxybenzoic acid **A28**
 2-(acetyloxy)benzoic acid 4-(acetylamino)phenyl ester **B33**
 (3 β ,6 β)-6-(acetyloxy)-3-(β -D-glucopyranosyloxy)-8,14-dihydroxybufa-4,20,22-trienolide **S10**
 (17 α)-17-(acetyloxy)-19-norpregn-4-en-20-yn-3-one, mixture with (17 α)-19-norpregn-1,3,5(10)-trien-20-yne-3,17-diol **N207**
 12-(acetyloxy)-14,15,20,21-tetradehydro-15,20-dihydro-8-hydroxy-4-methyl-11,16-dioxoseneconanium, (8 ϵ ,12 β ,14*Z*)- **C355**
 (acetyloxy)tributylstannane **T213**
 acetyl peroxide **D66**
 acetylphosphoramidothioic acid *O,S*-dimethyl ester **A5**
 2-acetylpropane **M244**
 β -acetylpropionic acid **L40**

acetylpropionyl **P40**
 acetylsalicylic acid **A28**
 7 α -acetylthio-3-oxo-17 α -pregn-4-ene-21,17 β -carb lactone **S108**
 1-acetyl-2-thiourea **A29**
N-acetyl thiourea **A29**
N-acetyltrimethylcolchicine acid, methyl ester **C384**
 Acibel **G14**
 acid ammonium carbonate **A165**
 Acid Blue 74 **I26**
 Acid Brilliant Green BS **C389**
 Acid Brilliant Scarlet 3R **C394**
 acid butyl phosphate **B237**
 acid lead arsenate **L13**
 Acidol **N12**
 Acid Sky Blue A **C411**
 acid-spar **F80**
 Acid Yellow 73 **C399**
 acifluorfen **A30**
 Acifon **A264**
 Acillin **A194**
 acinitrazole **A31**
 Aciron **I133**
 aclonifen **A32**
 Acna Naphthol **N19**
 ACNQ **Q8**
 acocantherin **O40**
 aconitine **A33**
 Acorit **H80**
 Acquit **C543**
 ACR 1139A **D362**
 Acrichin **M55**
 acridine **A34**
 3,6-acridinediamine, monohydrochloride **P280**
 Acridine Orange Base **C421**
 Acrinamione **M55**
 Acritene **F97**
 acroleic acid **A42**
 acrolein **A35**
 acrolein acetal **A39**
 acrolein diacetate **A37**
 acrolein dibromide **A38**
 acrolein diethyl acetal **A39**
 acrolein dimer **A36**
 acromycine **A40**
 acronine **A40**
 acronycine **A40**
 acrylaldehyde **A35**
 acrylaldehyde diethyl acetal **A39**
 acrylamide **A41**
 Acryl Brilliant Green B **M9**
 acrylic acid **A42**
 acrylic acid, 3-*p*-anisoyl-3-bromo-, sodium salt **C547**
 acrylic acid, butyl ester **B238**
 acrylic acid chloride **A44**
 acrylic acid, 2,2-dimethyltrimethylene ester **N41**
 acrylic acid, hexyl ester **H78**

acrylic acid, isobutyl ester **I88**
 acrylic acid, methyl ester **M153**
 acrylic acid, 1-methyltrimethylene ester **B206**
 acrylic acid, neopentetetrayl ester **P36**
 acrylic acid, oxydiethylene ester **D302**
 acrylic acid, tetraester with pentaerythritol **P36**
 acrylic acid, tetramethylene ester **B207**
 acrylic aldehyde **A35**
 acrylic amide **A41**
 acrylic chloride **A44**
 Acryloid A-30 **P226**
 acrylonitrile **A43**
 acryloyl chloride **A44**
 acrylyl chloride **A44**
 Acsius **P56**
 Actane **H51**
 Actellic **P210**
 Acti-Dione **C513**
 Actifen **I2**
 Actilin **N36**
 actinomycin C **A45**
 Actinomycin C1 **A46**
 actinomycin D **A46**
 Activ-8 **P60**
 activated aluminium oxide **A103**
 Active 2 **C381**
 Activol **G14**
 Activox B **Z12**
 Actril **I59**
 Actrilawn **I59**
 Actylol **E141**
 Acytol **E141**
 adamantane **A47**
 Adamycin **O64**
 Adeka Carpol MH500 **P218**
 Adeka Hypote **S74**
 Ademine **T203**
 adenine, *N*⁶-furfuryl- **K11**
 adepsine oil **M333**
 adermin **P358**
 Aderoxin **P359**
 Adhere **M196**
 Adine **D594**
 adipic acid **A48**
 adipic acid, bis[2-(2-butoxyethoxy)ethyl] ester **D139**
 adipic acid, bis(2-hexyloxyethyl) ester **B129**
 adipic acid, dibutyl ester **D140**
 adipic acid, diisobutyl ester **D351**
 adipic acid, diisopropyl ester **D357**
 adipic acid dinitrile **A49**
 adipic acid, dioctyl ester **D513**
 adipic acid monoethyl ester **E136**
 adipic ketone **C525**
 adiponitrile **A49**
 Adiposon **D315**
 ADK STAB OT-1 **D524**
 Admire **I8**
 Adogeren 142 **S111**
 Adol **L34**
 Adol 61 NF **S113**
 Adonal **P79**
 1-(+)-adrenaline **A50**
 D-adrenaline **A50**
 L-adrenaline **A51**
 Adriablastina **D597**
 Adriablastina **D596**
 Adriacin **D597**
 adriamycin (former generic name) **D596**
 Adriamycin hydrochloride **D597**
 Adroyd **O62**
 Adrucil **F79**
 Adulsin **M185**
 Advance TJP360 **T339**
 Advantage **C83**
 ADX 100 **D591**
 aero-cyanamid **C29**
 Aeronesin **G47**
 aeropax **P222**
 Aerosol OT-70 PG **D583**
 Aerovan **D258**
 Aethon **T286**
 aethynodiolum diaceticum **E182**
 Aetina **E69**
 AF-2 **F132**
 Afalon **L50**
 AFBI **A53**
 Affix **C141**
 Afidan **E19**
 Afidan **E20**
 Afidrex **D376**
 Afilene **B223**
 Afitox **M111**
 aflatoxicol **A52**
 aflatoxin B **A53**
 aflatoxin B₁ **A53**
 aflatoxin B₂ **A54**
 aflatoxin G₁ **A55**
 aflatoxin G₂ **A56**
 aflatoxin M₁ **A57**
 aflatoxin R₀ **A52**
 Aflix **F105**
 Aflon **P232**
 Afracid **C63**
 Afraclor **C298**
 Afrathion **M11**
 Afrisect **C542**
 Afrodane **D505**
 Afugan **P350**
 A.F. Violet No 1 **B101**
 Agaclor **E19**
 agar **A58**
 agar-agar **A58**
 Agarin **M356**
 Agarine **M356**

agaritine **A59**
 agate **Q1**
 Ageflex BGE **B259**
 Ageflex HDDA **H61**
 Ageflux-n-HA **H78**
 Age Rite Powder **P124**
 Agerite Resin D **A16**
 Agermin **P305**
 Agilene **P224**
 Agostilben **S116**
 Agrenocap **D505**
 Agrex K **D261**
 Agrex R **D376**
 Agria 1060 **P149**
 Agrian **M11**
 Agri-bloc **C238**
 Agricorn **M32**
 agricultural limestone **C25**
 Agricur **F23**
 Agrijet **E72**
 Agrimer VEMA-H-240 **M317**
 Agrimet **P145**
 Agrisan **E40**
 Agrisil **T253**
 Agrisynt MVE **M317**
 Agritoluron **C298**
 Agritox **T253**
 Agritrel **E63**
 Agrocapt **C59**
 Agrofos **M343**
 Agrosol **M251**
 Ahco DFS100 **P229**
 Aikylate P1 **P100**
 Aimchlor **B196**
 Aimcocyper **C542**
 Aimcosystox **O57**
 Aimocron **M343**
 Airvol 103 **P234**
 Aisemide **F112**
 Aithulphos **A263**
 Aizen Magenta **M1**
 Ajax **C40**
 Akrochem DPG **D545**
 Akrochem TDEC **E174**
 Akrochem TETD **D565**
 Akrochem TMTD **T147**
 Akroform ETU-22 PM **E122**
 Aktikon **A252**
 Aktisal **O46**
 alachlor **A60**
 alamine 11 **O28**
 Alamine 7 **S111**
 Alamo **P306**
 L-alanine, *N*-benzoyl-*N*-(3,4-dichlorophenyl)ethyl ester
B84
 alanycarb **A61**
 Albagel premium USP444 **B39**
 Albisal **H120**
 albocarbon **N9**
 Albone **H103**
 albuterol **S3**
 Alcance **C543**
 Alcobam NM **S64**
 alcohol C-8 **O13**
 alcohol C-9 **N195**
 Alcosolve 2 **P297**
 Alcotox 75L **P234**
 Alcox **P225**
 Aldacide **P8**
 aldehyde C-9 **N192**
 aldehyde C7 **H19**
 aldehydecollidine **E163**
 aldehydine **E163**
 Alden **P206**
 aldicarb **A62**
 Aldinamide **P348**
 aldol **A63**
 Aldomet **M208**
 aldoxime **A9**
 aldoxycarb **A64**
 aldrin **A65**
 Alexan **C546**
 Alfacron **I50**
 Alfacron **A259**
 Alfadex **P354**
 alfa-interferon **I39**
 Alfamat **C109**
 Alferon **I39**
 Alficon **A259**
 Alfimid **G22**
 Alflorone **F63**
 Alfol 18 NF **S113**
 Alfrocip **C59**
 algaroba **L57**
 Algimycin 200 **P116**
 Algrol **L50**
 Aliette **F108**
 Align **A258**
 Aliphat No.4 **L8**
 Alirox **E40**
 alkali lignin **L42**
 alkanes (C₂₂₋₂₆), chlorinated **C134**
 alkanes, chlorinated **C133**
 Alkanolamine **D388**
 Alkarsodyl **S63**
 Alkathene **P224**
 Alkeran **M49**
 Alkiron **M312**
 Alkofen B **T211**
 alkyl(C₁₄-C₁₆)dimethylbenzylammonium chloride **A66**
N-alkyl(C₈-C₁₈)dimethylbenzylammonium chloride **B41**
N-alkyl(C₈-C₁₈)dimethyl-3,4-dichlorobenzylammonium
 chloride **A67**
N-alkyl-1,3-propanediamine **T4**

all-*trans*-capsorubin **C57**
 all-*trans*-1,5,9-cyclododecatriene **C503**
 Allerdryl **D537**
 Allergan **D537**
 allethrin **A68**
 allidochlor **A69**
 Allied GC 5606 **M311**
 Allirem **M14**
 Allisan **D260**
 All Muis Kill **C109**
 allocaine **P273**
 allomaleic acid **F115**
 Allopren **C262**
 allopurinol **A70**
 alloxymedon sodium **A71**
 alloxym-sodium **A71**
 Ally **M328**
 allyl acetate **A72**
 allyl alcohol **A73**
 allyl alcohol oxide **G28**
 allyl aldehyde **A35**
 allylamine **A74**
 4-allylanisole **A75**
p-allylanisole **A75**
 allyl bromide **A76**
 allyl butanoate **A77**
 allyl butyrate **A77**
 allyl caprylate **A89**
 allylcarbinol **B219**
 allylcatechol methylene ether **S2**
 allyl chloride **A78**
 allyl chlorocarbonate **A79**
 allyl chloroformate **A79**
 allyl cinnamate **A80**
 allyl cyclohexane propionate **A81**
 allyl cyclohexylpropionate **A81**
 allyl-3-cyclohexyl propionate **A81**
 allyl- β -cyclohexyl propionate **A81**
 3-allylcyclohexyl propionate **A81**
 1-allyl-3,4-dimethoxybenzene **M223**
 4-allyl-1,2-dimethoxybenzene **M223**
 1-allyl-2,3-dimethoxy-4,5-(methylenedioxy)benzene **D366**
 1-allyl-2,5-dimethoxy-3,4-(methylenedioxy)benzene **A230**
 1-allyl-1-(3,7-dimethyloctyl)piperidinium bromide **P206**
 allyldioxybenzene methylene ether **S2**
 allylene **P338**
 allyl-2,3-epoxypropyl ether **A84**
 allyl ether **D71**
 allyl ethyl ether **A82**
 allyl formate **A83**
 allyl glycidyl ether **A84**
 allyl guaiacol **E187**
 allyl hexahydrophenyl propionate **A81**
 allylidene acetate **A37**
 allylidene diacetate **A37**
 allyl iodide **A85**
 allylisopropylacetamide **A86**
 allyl isorhodanide **A87**
 allyl isosulfocyanate **A87**
 allyl isothiocyanate **A87**
 allyl isovalerate **A88**
 allyl isovalerianate **A88**
 4-allyl-2-methoxyphenol **E187**
 5-allyl-5-(1-methylbutyl)barbituric acid **Q3**
 4-allyl-1,2-methylenedioxybenzene **S2**
 allyl octanoate **A89**
 allyl octylate **A89**
 1-(allyloxy)-2,3-epoxypropane **A84**
 1-[*o*-(allyloxy)phenoxy]-3-(isopropylamino)-2-propanol **O52**
 (allyloxy)propanol **P328**
 allyl phenoxyacetate **A90**
 allyl phenylacetate **A91**
 allyl- β -phenylacrylate **A80**
 allyl-3-phenylpropenoate **A80**
 allyl propyl disulfide **A92**
m-allylpyrocatechin methylene ether **S2**
 allyl sulfocarbamide **A93**
 allyl thiocarbamide **A93**
 allyl thiocarbonimide **A87**
 allylthiourea **A93**
 1-allyl-2-thiourea **A93**
 allyl α -toluate **A91**
 allyl trichloride **T264**
 allyl trichlorosilane **A94**
 4-allylveratrole **M223**
 aloe emodin **A95**
 Aloten **C132**
 Alperox C **L9**
 Alphaguard **C543**
 alpha-interferon **I39**
 Alphakil **C109**
 Alpha W6 Pharma Grade **C500**
 Alphos **D258**
 Alrheumun **K10**
 Alsol **E54**
 Altabactina **F122**
 Altacite **H108**
 Alta Musepulver **C109**
 Altene **T249**
 Altomix **D566**
 Altozar **H106**
 Altuglas **P226**
 alum **A105**
 alum flour **A105**
 alumina **A103**
 α -alumina **A103**
 β -alumina **A103**
 γ -alumina **A103**
 aluminium **A96**
 aluminium bromide **A97**
 aluminium carbide **A98**
 aluminium chloride **A99**
 aluminium fibre **A96**

aluminium flake **A96**
 aluminium hydride **A100**
 aluminium isopropoxide **A101**
 aluminium isopropylate **A101**
 aluminium lithium hydride **L53**
 aluminium magnesium carbonate hydroxide hydrate **H108**
 aluminium nitrate nonahydrate **A102**
 aluminium oxide **A103**
 aluminium phosphide **A104**
 aluminium potassium sulfate **A105**
 aluminium powder **A96**
 aluminium resin **A106**
 aluminium sesquioxide **A103**
 aluminium silicate hydroxide **K2**
 aluminium sulfate **A107**
 aluminium tribromide **A97**
 aluminium trichloride **A99**
 aluminium trihydride **A100**
 α -aluminium trihydride **A100**
 aluminium triisopropoxide **A101**
 aluminium tris(ethyl phosphite) **F108**
 aluminium tris(*O*-ethyl phosphorate) **F108**
 aluminum **A96**
 alvit **D276**
 Alvora **N3**
 alvyl **P234**
 Alzodef **C479**
 Amacel Developed Navy SD **D95**
 Amacid Brilliant Blue **I26**
 Amangan **M21**
 Amanthrene Golden Yellow **C428**
 Amaranth **A108**
 Amarthol Fast Red GL Base **M261**
 Amarthol Fast Scarlet GG Base **D180**
 Amasil **F104**
 Amaze **I103**
 AMBEN **A117**
 amber acid **S128**
 Amber musk **M357**
 Ambilhar **N62**
 ambush **A62**
 Amdro **H86**
 Americaine **B55**
 American Cyanamid 18133 **T135**
 American Cyanamid 47031 **P151**
 American Cyanamid 18706B/77 **E71**
 amethopterin **M128**
 L-(+)-amethopterin **M128**
 amethyst **Q1**
 Ametrex **A109**
 ametryn **A109**
 Ametycine **M336**
 Amex **B232**
 Amexine **B232**
 Amfepramone **D316**
 Amiben **C110**

Amicol **S110**
 amide C₂ **A10**
 amides, coco, *N,N*-bis(hydroxyethyl) **C381**
 Amidex 1285 **C381**
 Amidex L-9 **L7**
N'-amidinosulfanilamide **S134**
 amidithion **A110**
 Amido-F acid **A135**
 amidopyrine **A154**
 amidosulfonic acid **S137**
 amidourea hydrochloride **S22**
 Amietol **E62**
 Amimycin **O29**
 Amine 8 D **D515**
 aminic acid **F104**
 aminitrozole **A31**
 aminoacetic acid **G36**
 4-amino-*N*-(aminoiminomethyl)benzenesulfonamide **S134**
 4-[[3-amino-5-[(aminoiminomethyl)methylamino]-1-oxopentyl]amino]-1-(4-amino-2-oxo-1(2*H*)-pyrimidinyl)-1,2,3,4-tetradeoxy- β -D-*erythro*-hex-2-enopyranuronic acid **B139**
 2-aminoaniline **P102**
 3-aminoaniline **P101**
 4-aminoaniline **P103**
m-aminoanisole **A214**
o-aminoanisole **A213**
p-aminoanisole **A215**
 2-aminoanthracenamine **A111**
 2-aminoanthracene **A111**
 β -aminoanthracene **A111**
 2-amino-9,10-anthracenedione **A112**
 2-aminoanthraquinone **A112**
 β -aminoanthraquinone **A112**
 4-aminoantipyrene **A113**
 4-amino-1-arabinofuranosyl-2-oxo-1,2-dihydropyrimidine **C546**
 4-amino-1- β -D-arabinofuranosylpyrimidin-2-(1*H*)-one **C546**
 4-aminoazobenzene **A114**
 2-amino-5-azotoluene **C424**
 4'-amino-2,3'-azotoluene **C424**
o-aminoazotoluene **C424**
m-aminobenzal fluoride **A118**
 aminobenzene **A209**
 (S)- α -aminobenzenepropanoic acid **P92**
p-aminobenzenesulfoguanidide **S134**
 5-*p*-aminobenzenesulfonamido)-3,4-dimethylisoxazole **S141**
 3-(*p*-aminobenzenesulfonamido)-2-phenylpyrazole **S139**
 1-aminobenzene-3-sulfonic acid **M97**
 2-aminobenzenesulfonic acid **A211**
 3-aminobenzenesulfonic acid **M97**
 4-aminobenzenesulfonic acid **S138**
 2-aminobenzoic acid **A115**
 3-aminobenzoic acid **A116**

4-aminobenzoic acid **A117**
m-aminobenzoic acid **A116**
o-aminobenzoic acid **A115**
p-aminobenzoic acid **A117**
 4-aminobenzoic acid, 2-(diethylamino)ethyl ester **P273**
p-aminobenzoic acid, ethyl ester **B55**
 2-aminobenzoic acid, 3-phenyl-2-propenyl ester **C347**
 3-aminobenzotrifluoride **A118**
p-aminobenzoyldiethylaminoethanol **P273**
o-aminobenzoylformic anhydride **I78**
 amino benzylpenicillin **A194**
 2-aminobiphenyl **A119**
 3-aminobiphenyl **A120**
 4-aminobiphenyl **A121**
m-aminobiphenyl **A120**
o-aminobiphenyl **A119**
p-aminobiphenyl **A121**
 5-amino-1-bis(dimethylamido)phosphoryl-3-phenyl-1,2,4-triazole **T202**
 5-amino-1,3-bis(2-ethylhexyl) hexahydro-5-methylpyrimidine **H75**
 aminobis(propylamine) **N208**
 1-aminobutane **B239**
 2-aminobutane **B240**
 (4-aminobutyl)diethoxymethylsilane **A122**
 4-amino-6-*tert*-butyl-3-(methylthio)-1,2,4-triazin-5(4*H*)-one **M326**
 aminocaproic lactam **C55**
 aminocarb **A123**
 2-amino- α -carboline **A1**
 2-amino-4-chloroaniline **C245**
 1-amino-2-chlorobenzene **C154**
 1-amino-3-chlorobenzene **C155**
 1-amino-4-chlorobenzene **C156**
m-aminochlorobenzene **C155**
o-aminochlorobenzene **C154**
 2-amino-5-chlorobenzoxazole **Z25**
 1-amino-3-chloro-2-methylbenzene **C292**
 2-amino-3-chloro-1,4-naphtholenedione **Q8**
 2-amino-3-chloro-1,4-naphthoquinone **Q8**
 1-amino-2-chloro-4-nitrobenzene **C220**
 2-amino-4-chlorophenol **A124**
 5-amino-4-chloro-2-phenylpyridazin-3(2*H*)-one **C131**
 2-amino-3-chlorotoluene **C297**
 2-amino-4-chlorotoluene **C296**
 2-amino-5-chlorotoluene **C294**
 2-amino-6-chlorotoluene **C292**
 4-amino-2-chlorotoluene **C293**
 4-amino-3-chlorotoluene **C291**
 2-amino-5-chlorotoluene hydrochloride **C295**
o-aminocinnamic acid **H118**
 3-amino-*p*-cresol, methyl ether **C455**
 aminocyclohexane **C514**
 O-2-amino-2-deoxy- α -D-glucopyranosyl-(1 \rightarrow 4)-O-[O]-2,6-diamino-2,6-dideoxy- β -L-idopyranosyl-(1 \rightarrow 3)- β -D-ribofuranosyl-(1 \rightarrow 5)]-2-deoxy-D-steptom **N38**
 aminodiacetic acid **I11**
 4-amino-3-((4'-((2,4-diaminophenyl)azo)(1,1'-biphenyl)-4-yl)azo)-5-hydroxy-6-(phenylazo)-2,7-naphthalenedisulfonic acid, disodium salt **C403**
 3-aminodibenzofuran **D114**
 1-amino-2,4-dibromo-9,10-anthracenedione **A125**
 1-amino-2,4-dibromoanthraquinone **A125**
 3-amino-2,5-dichlorobenzoic acid **C110**
 [(4-amino-3,5-dichloro-6-fluoro-2-pyridinyl)oxy]acetic acid **F88**
 (\pm)-5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-[(trifluoromethyl)sulfinyl]-1*H*-pyrazole-3-carbonitrile **F33**
 (\pm)-5-amino-1-(2,6-dichloro- α,α,α -trifluoro-*p*-tolyl)-4-trifluoromethylsulfinylpyrazole-3-carbonitrile **F33**
 aminodicyclohexane **D265**
 4-amino-*N,N*-diethylaniline **D313**
p-aminodiethylaniline **D313**
 4-amino-4,5-dihydro-3-methyl-6-phenyl-1,2,4-triazin-5-one **M95**
N-[4-[[[(2-amino-1,4-dihydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]-L-glutamic acid **F96**
 2-amino-1,7-dihydro-6*H*-purin-6-one **G50**
 4-aminodimethylaniline **D448**
p-aminodimethylaniline **D448**
 1-amino-2,3-dimethylbenzene **D395**
 1-amino-2,4-dimethylbenzene **D396**
 1-amino-2,5-dimethylbenzene **D397**
 1-amino-3,5-dimethylbenzene **D400**
 2-amino-1,3-dimethylbenzene **D398**
 2-amino-1,4-dimethylbenzene **D397**
 4-amino-1,2-dimethylbenzene **D399**
 4-amino-1,3-dimethylbenzene **D396**
 3-amino-1,4-dimethyl- γ -carboline **T364**
 4-amino-6-(1,1-dimethylethyl)-3-(methylthio)-1,2,4-triazin-5(4*H*)-one **M326**
 2-amino-3,4-dimethylimidazo[4,5-*f*]quinoline **M45**
 2-amino-3,8-dimethylimidazo[4,5-*f*]quinoxaline **M46**
 4-amino-*N*-(3,4-dimethyl-5-isoxazolyl)benzenesulfonamide **S141**
 4-amino-2,3-dimethyl-1-phenyl-3-pyrazolin-5-one **A113**
 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole **T364**
 4-amino-*N*-(4,6-dimethyl-2-pyrimidinyl)benzenesulfonamide **S133**
 2-amino-4,6-dinitrophenol **A126**
 4-aminodiphenyl **A121**
p-aminodiphenyl **A121**
 4-aminodiphenylamine **P128**
p-aminodiphenylimide **A114**
 2-aminodipyrido[1,2-*a*:3',2'-*d*]imidazole **G20**
 aminoethane **E90**
 1-aminoethane **E90**
 aminoethanoic acid **G36**
 2-aminoethanol **E62**
 2-(2-aminoethoxy)ethanol **A127**
 β -aminoethyl alcohol **E62**
 β -aminoethylamine **E114**

N-(2-aminoethyl)-*N'*-[2-[(2-aminoethyl)amino]ethyl]-1,2-ethanediamine **T65**
 4-aminoethylbenzene **E94**
 β -(aminoethyl)benzene **P69**
 4-(2-aminoethyl)-1,2-benzenediol **D595**
 α -(1-aminoethyl)benzenemethanol hydrochloride **N203**
 3-amino-9-ethylcarbazole **A128**
 3-amino-*N*-ethylcarbazole **A128**
 aminoethylene **A266**
N-(2-aminoethyl)ethane-1,2-diamine **D303**
 1-amino-2-ethylhexane **E132**
 3-(2-aminoethyl)indole **T367**
 4-(2-aminoethyl)phenol **T375**
p- β -aminoethylphenol **T375**
N-aminoethylpiperazine **A129**
N-(β -aminoethyl)piperazine **A129**
 4-(2-aminoethyl)pyrocatechol **D595**
 4-amino-4'-fluorodiphenyl **F57**
 Aminoform **H57**
 6-aminohexanoic acid, cyclic lactam **C55**
 α -aminohydrocinnamic acid **P92**
 3-amino-4-hydroxyaniline **D81**
 2-amino-1-hydroxybenzene **A142**
 3-amino-1-hydroxybenzene **A143**
 4-amino-1-hydroxybenzene **A144**
 α -amino-*p*-hydroxybenzylpenicillin **A192**
D-(-)- α -amino-*p*-hydroxybenzyl penicillin **A192**
 2-amino-3-hydroxybutanoic acid **T152**
 2-amino-3-hydroxybutyric acid **T152**
 α -amino- β -hydroxybutyric acid **T152**
 2-amino-2-(hydroxymethyl)-1,3-propanediol **T356**
 3-amino-4-hydroxynitrobenzene **A138**
 4-amino-3-hydroxynitrobenzene **A139**
 α -amino-*p*-hydroxyphenylacetamido]penicillanic acid **A192**
 2-amino-3-hydroxypropanoic acid **S24**
 2-amino-3-hydroxypropionic acid **A260**
 2-amino-6-hydroxypurine **G50**
N-(*p*-[(2-amino-4-hydroxypyrimido[4,5-*b*]pyrazin-6-yl)methylamino]benzoyl)-glutamic acid **F96**
 2-aminohypoxanthine **G50**
 2-amino-3-indolylpropanoic acid **T369**
 α -amino- β -(3-indolyl)propionic acid **T369**
 3-aminoiodobenzene **I43**
 4-aminoiodobenzene **I44**
m-aminoiodobenzene **I43**
 2-aminoisobutane **B241**
 α -aminoisopropyl alcohol **A148**
 α -aminoisovaleric acid **V6**
DL- α -aminoisovaleric acid **V5**
 aminomercuric chloride **M66**
 aminomesitylene **T305**
 2-aminomesitylene **T305**
 aminomethane **M154**
 1-amino-4-methoxybenzene **A215**
 1-amino-2-methoxy-5-methylbenzene **C455**
 2-amino-1-methoxy-4-nitrobenzene **M142**
 3-amino-4-methoxynitrobenzene **M142**
 2-amino-6-methoxypurine **M139**
 3-amino-4-methoxytoluene **C455**
 4-amino-2-methylaniline **D88**
 2-amino-4-methylanisole **C455**
 1-amino-2-methyl-9,10-anthracenedione **A130**
 1-amino-2-methylanthraquinone **A130**
 3-amino-1-methyl- γ -carboline **T365**
 2-amino-6-methyldipyrido[1,2-*a*:3',2'-*d*]imidazole **G19**
 4-amino-10-methylfolic acid **M128**
 4-[3-amino-5-(1-methylguanidino)-valeramido]-1-(4-amino-2-oxo-1(2*H*)-pyrimidinyl-1,2,3,4-tetradexy- β -*D*-erythro-hex-2-enopyranuronic acid **B139**
 5-(aminomethyl)-3(2*H*)-isoxazalone **M356**
 4-amino-*N*-(5-methyl-3-isoxazolyl)benzenesulfonamide **S136**
 5-aminomethyl-3-isoxazole **M356**
d-2-amino-3-methylpentanoic acid **I108**
 2-amino-1-methyl-6-phenylimidazole[4,5-*b*]pyridine **P144**
 4-amino-3-methyl-6-phenyl-1,2,4-triazin-5(4*H*)-one **M95**
 2-amino-2-methylpropane **B241**
 4-amino-*N*-methylpteroylglutamic acid **M128**
 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole **T365**
 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methylthiazolium chloride **T112**
 4-amino-3-methyltoluene **D396**
 3-aminomethyl-3,5,5-trimethylcyclohexylamine **I111**
d- α -amino- β -methylvaleric acid **I108**
 1-aminonaphthalene **N23**
 2-aminonaphthalene **N24**
 1-aminonaphthalene-4-sulfonic acid **A132**
 2-amino-1-naphthalenesulfonic acid **A131**
 2-aminonaphthalene-1-sulfonic acid **A131**
 4-aminonaphthalene-1-sulfonic acid **A132**
 5-amino-2-naphthalenesulfonic acid **A133**
 5-aminonaphthalene-2-sulfonic acid **A133**
 6-amino-2-naphthalenesulfonic acid **A134**
 6-aminonaphthalene-2-sulfonic acid **A134**
 7-amino-2-naphthalenesulfonic acid **A135**
 7-aminonaphthalene-2-sulfonic acid **A135**
 8-aminonaphthalene-2-sulfonic acid **A136**
 8-amino-2-naphthalenesulfonic acid **A136**
 2-amino-4-nitroaniline **N134**
 4-amino-2-nitroaniline **N133**
 2-amino-4-nitroanisole **M142**
 2-amino-5-nitroanisole **M141**
 4-amino-3-nitroanisole **M143**
 1-amino-2-nitrobenzene **N74**
 1-amino-3-nitrobenzene **N75**
 1-amino-4-nitrobenzene **N76**
p-aminonitrobenzene **N76**
 2-amino-4-nitrobenzoic acid **N80**
 2-amino-5-(5-nitro-2-furyl)-1,3,4-thiadiazole **A137**
 5-amino-2-(5-nitro-2-furyl)-1,3,4-thiadiazole **A137**
 1-amino-3-nitro-4-methylbenzene **M262**
 2-amino-4-nitrophenol **A138**
 2-amino-5-nitrophenol **A139**

4-amino-2-nitrophenol **A140**
 aminonitrothiazole **A141**
 2-amino-5-nitrothiazole **A141**
 aminonitrothiazolium **A141**
 1-aminooctadecane **S111**
 1-aminopentadecane **P33**
 1-aminopentane **P47**
 aminophen **A209**
 4-aminophenazone **A113**
 4-aminophenazone **A154**
 2-aminophenetole **P71**
 4-aminophenetole **P72**
p-aminophenetole **P72**
 2-aminophenol **A142**
 3-aminophenol **A143**
 4-aminophenol **A144**
m-aminophenol **A143**
o-aminophenol **A142**
m-aminophenol methyl ether **A214**
 7-(*D*- α -aminophenylacetamido)desacetoxycephalosporanic acid **C100**
 (4-aminophenyl)arsonic acid, sodium salt **S43**
 3-aminophenylmethane **T184**
 2-[(4-aminophenyl)methyl]benzamine **M217**
 2-(4-aminophenyl)-6-methylbenzothiazole **A145**
 2-(4-aminophenyl)-6-methyl-7-benzothiazolesulfonic acid **A146**
 2-(4-aminophenyl)-6-methyl-7-benzothiazolylsulfonic acid **A146**
 (\pm)-2-amino-1-phenyl-1-propanol hydrochloride **N203**
 1-(4-aminophenyl)-1-propanone **A149**
p-aminophenylpropanone **A149**
 4-amino-*N*-(1-phenyl-1*H*-pyrazol-5-yl)benzenesulfonamide **S139**
 3-(*p*-aminophenylsulfonamido)-5-methylisoxazole **S136**
o-aminophenylsulfonic acid **A211**
p-aminophenylsulfonic acid **S138**
 5-amino-3-phenyl-1,2,4-triazole-1-yl-*N,N,N',N'*-tetramethylphosphodiamide **T202**
 aminophylline **A147**
 aminopropane **P323**
 1-aminopropane **P323**
 2-aminopropane **I121**
 1-amino-2-propanol **A148**
 1-aminopropan-2-ol **A148**
 3-aminopropene **A74**
 4'-aminopropiophenone **A149**
p-aminopropiophenone **A149**
 β -aminopropylbenzene **A193**
 3-aminopropyl-diethylamine **D290**
 3-aminopropyl-dimethylamine **D392**
 3-aminopropylene **A74**
 aminopteridine **A150**
 2-amino-4(1*H*)-pteridinone **P345**
 2-amino-4(3*H*)-pteridinone **P345**
 aminopterin **A150**
 amino-2-pyridine **A151**
 amino-3-pyridine **A152**
 amino-4-pyridine **A153**
 2-aminopyridine **A151**
 3-aminopyridine **A152**
 4-aminopyridine **A153**
 α -aminopyridine **A151**
 γ -aminopyridine **A153**
m-aminopyridine **A152**
o-aminopyridine **A151**
p-aminopyridine **A153**
 2-amino-1*H*-pyrido[2,3-*b*]indole **A1**
 2-amino-9*H*-pyrido[2,3-*b*]indole **A1**
 4-amino-*N*-2-pyrimidinylbenzenesulfonamide **S132**
 aminopyrine **A154**
 4-amino-1- β -*D*-ribofuranosyl-1,3,5-triazin-2(1*H*)-one **A257**
 4-amino-1- β -*D*-ribofuranosyl-s-triazin-2(1*H*)-one **A257**
 4-aminosemicarbazide **C69**
 aminosidin **N38**
 Aminosin **A93**
 1-amino-4-sulfonaphthalene **A132**
 5-aminosulfonyl-4-chloro-2-[(2-furanylmethyl)amino]benzoic acid **F112**
 1-aminothiourea **T144**
N-aminothiourea **T144**
 aminotoluene **B90**
 2-aminotoluene **T185**
 3-aminotoluene **T184**
 4-aminotoluene **T187**
 3-amino-*p*-toluidine **D87**
 5-amino-*o*-toluidine **D87**
 aminotriacetic acid **N70**
 aminotriazole **A160**
 3-amino-1*H*-1,2,4-triazole **A160**
 3-amino-s-triazole **A160**
 4-amino-3,5,6-trichloropicolinic acid **P182**
 4-amino-3,5,6-trichloropyridine-2-carboxylic acid **P182**
 10-[(3-amino-2,3,6-trideoxy- α -*L*-lyxo-hexapyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-5,12-naphthacenedione hydrochloride **D597**
 (8*S*-*cis*)-10-[(3-amino-2,3,6-trideoxy- α -*L*-lyxo-hexapyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-5,12-naphthacenedione **D596**
 1-amino-2,4,5-trimethylbenzene **T304**
 5-amino-1,3,3-trimethyl-cyclohexanemethylamine **I111**
 11-aminoundecanoic acid **A155**
 aminouracil mustard **B119**
 aminourea hydrochloride **S22**
 2-amino-1,4-xylene **D397**
 4-amino-1,3-xylene **D396**
 1,2-aminozophenylene **B78**
 Amitex B **H103**
 amiton **A156**
 amiton hydrogen oxalate **A157**
 amiton oxalate **A157**

amitraz **A158**
 amitriptyline **A159**
 Amitrol-100 **N144**
 amitrole **A160**
 amizol **A160**
 Ammoidin **M129**
 ammonia **A161**
 ammonia water **A176**
 ammonioformaldehyde **H57**
 ammonium acetate **A162**
 ammonium acid arsenate **A163**
 ammonium acid difluoride **A175**
 ammonium amidosulfonate **A184**
 ammonium aminoformate **A167**
 ammonium (\pm)-2-amino-4-
 (hydroxymethylphosphinyl)butanote **G18**
 ammonium arsenate **A163**
 ammonium benzoate **A164**
 ammonium bicarbonate **A165**
 Ammonium bichromate(vi) **A172**
 ammonium bifluoride **A175**
 ammonium bisulfite **A166**
 ammonium borofluoride **A189**
 ammonium carbamate **A167**
 ammonium carbamate **A167**
 ammonium carbazate **A182**
 ammonium carbonate **A168**
 ammonium, [9-(*o*-carboxyphenyl)-6-(diethylamino)-3*H*-
 xanthen-3-ylidene]diethyl-, chloride **R9**
 ammonium chloride **A169**
 ammonium chloroplatinate(iv) **A170**
 ammonium chloroplatinate **A170**
 ammonium chromate **A171**
 ammonium chromate(vi) **A171**
 ammonium dichromate **A172**
 ammonium, 16-(diethylamino)-9-(2,4-disulfophenyl)-3*H*-
 xanthen-3-ylidene]diethyl-, hydroxide, inner salt,
 sodium salt **C396**
 ammonium, [[4-(*p*-(diethylamino)- α -phenylbenzylidene]-
 2,5-cyclohexadien-1-ylidene]diethyl-, sulfate(1:1) **C400**
 ammonium ethyl (aminocarbonyl)phosphonate **F107**
 ammonium ethyl carbamoylphosphonate **F107**
 ammonium, (ethyl)[(4-(*p*-[(ethyl-*m*-sulfobenzyl)amino]- α -(*o*-
 sulfophenyl)benzylidene]2,5-cyclohexadien-1-
 ylidene)(*m*-sulfobenzyl)-, hydroxide, inner salt,
 disodium salt **C411**
 ammonium ferrous sulfate **I67**
 ammonium fluoride **A173**
 ammonium fluoroborate **A189**
 ammonium fluorosilicate **A174**
 ammonium fluosilicate **A174**
 ammonium hexachloroplatinate(iv) **A170**
 ammonium hexafluorosilicate **A174**
 ammonium-DL-homoalanin-4-yl(methyl)phosphinic acid
 G18
 ammonium hydrogen carbonate **A165**
 ammonium hydrogen difluoride **A175**
 ammonium hydrogen fluoride **A175**
 ammonium hydrogen sulfite **A166**
 ammonium hydroxide **A176**
 ammonium hyposulfite **A191**
 ammonium metavanadate **A177**
 ammonium monosulfide **A186**
 ammonium muriate **A169**
 ammonium nickel sulfate **N45**
 ammonium nitrate **A178**
 ammonium *N*-nitrosophenylhydroxylamine **C476**
 ammonium oxalate **A179**
 ammonium perfluorooctanoate **A180**
 ammonium peroxydisulfate **A181**
 ammonium persulfate **A181**
 ammonium picrate **A182**
 ammonium picronitrate **A182**
 ammonium platinic chloride **A170**
 ammonium polysulfide **A183**
 ammonium rhodanate **A190**
 ammonium rhodanide **A190**
 ammonium saltpeter **A178**
 ammonium silicofluoride **A174**
 ammonium sulfamate **A184**
 ammonium sulfamidate **A184**
 ammonium sulfate **A185**
 ammonium sulfide **A186**
 ammonium sulfite **A187**
 ammonium sulfocyanate **A190**
 ammonium sulfocyanide **A190**
 ammonium tartrate **A188**
 ammonium tetrafluoroborate **A189**
 ammonium thiocyanate **A190**
 ammonium thiosulfate **A191**
 ammonium threonate **A188**
 ammonium trisulfide **A183**
 ammonium vanadate **A177**
 Amobarbital **A204**
 amorphous: diatomaceous earth **S29**
 amorphous silica **D97**
 Amorthol Fast Red B Base **M141**
 Amotril **C358**
 amoxycillin **A192**
 Ampen **A194**
 Ampfepramone **D315**
 amphetamine **A193**
 ampicillin **A194**
 ampyrone **A113**
 AMS **A184**
 Amso H-SB **N5**
 amsonic acid **D85**
 amudane **G46**
 Amuno **I35**
 amyl acetate **A195**
n-amyl acetate **A195**
sec-amyl acetate **P46**
tert-amyl acetate **A196**
 amylacetic ester **A195**

amyl alcohol **P41**
n-amyl alcohol **P41**
tert-amyl alcohol **M173**
n-amylamine **P47**
 amyl butyrate **A197**
m-amyl butyrate **A197**
 amylcarbinol **H65**
 amyl chloride **A198**
 amyl-3-cresol **A199**
 amyl-*m*-cresol **A199**
 6-amyl-*m*-cresol **A199**
 6-*n*-amyl-*m*-cresol **A199**
 2-*sec*-amyl-4,6-dinitrophenol **D509**
 amylenes **A200**
 α -*n*-amylenes **P43**
 amylenes hydrate **M173**
 amyl ether **P48**
 amyl ethyl ketone **E91**
 amyl mercaptan **A201**
 amylmetacresol **A199**
 amyl methyl alcohol **M277**
 amyl methyl ketone **H23**
 amyl nitrate **A202**
 1-amyl-1-nitrosourea **A203**
N-amyl-*N*-nitrosourea **A203**
 amylobarbitone **A204**
 Amylol **P41**
 β -amylose **C97**
 4-*tert*-amylphenol **A205**
p-*tert*-amylphenol **A205**
 amyl phthalate **D534**
 amyl propionate **P49**
 amyltrichlorosilane **A206**
 amylvinylcarbinol **O18**
 Anadrol **O62**
 Anadurm Orange AE 110% **C390**
 anaesthetic ether **D304**
 Analexin **P140**
 Analud **F29**
 anasterone **O62**
 Anatola **R7**
 ancymidol **A207**
 Andricite **C44**
 androlin **T38**
 androsol **T38**
 androst-4-en-17 β -ol-3-one **T38**
 Anelda **B243**
 Anestacon **L43**
 ANF **N13**
 Anglislite **L30**
 An gravid **O41**
 anhydro-4,4'-bis(diethylamino)triphenylmethanol-2'',4''-disulfonic acid, monosodium salt **C386**
 anhydrone **M7**
 anhydrous aluminium sulfate **A107**
 anhydrous brucine **B191**
 anhydrous chloral **C107**
 anhydrous gypsum **C44**
 anhydrous hydriodic acid **H102**
 anhydrous hydrobromic acid **H98**
 anhydrous hydrochloric acid **H99**
 anhydrous hydrofluoric acid **H101**
 anhydrous magnesium perchlorate **M7**
 anhydrous sulfate of lime **C44**
 anilazine **A208**
 Anilid **P295**
 aniline **A209**
 aniline, 2,3-dichloro- **D178**
 aniline, 2,4-dichloro- **D179**
 aniline, 2,5-dichloro **D180**
 aniline, 2,6-dichloro- **D181**
 aniline, 3,4-dichloro- **D182**
 aniline, *N,N*-diethyl- **D291**
 Aniline Green **C400**
 aniline hydrochloride **A210**
 aniline, 4,4-(imidocarbonyl)bis(*N,N*-dimethyl)- **A254**
 aniline oil **A209**
 aniline salt **A210**
 aniline-2-sulfonic acid **A211**
 aniline-4-sulfonic acid **S138**
 aniline-*m*-sulfonic acid **M97**
o-aniline sulfonic acid **A211**
 Aniline Yellow **A114**
 anilinium chloride **A210**
 anilinobenzene **D540**
 anilinoethane **E95**
 anilinomethane **M156**
 2-anilinonaphthalene **P124**
 anilino-*o*-sulfonic acid **A211**
 anilofos **A212**
 Animag **M6**
 animal galactose factor **O34**
 Animert **T98**
 2-anisidine **A213**
 3-anisidine **A214**
 4-anisidine **A215**
m-anisidine **A214**
o-anisidine **A213**
p-anisidine **A215**
o-anisidine nitrate **M142**
 anisole **A216**
 anisole, 3,5-dichloro- **D186**
 4-anisoyl chloride **A217**
p-anisoyl chloride **A217**
m-anisylamine **A214**
p-anisylamine **A215**
p-anisyl chloride **A217**
 Anovlar **N207**
 Anovlar 21 **N204**
 anprolene **E120**
 Anquil **R3**
 Ansar 170 **M355**
 Ansol E-121 **D381**
 Antabuse **D565**

Antagothyroil **T145**
 Anten **F85**
 Antergon **M14**
 anthanthren **D119**
 anthanthrene **D119**
 Anthio **F105**
 Anthion **P261**
 Anthium dioxide **C136**
 Anthonox **O57**
 anthracene **A218**
 2-anthracenecarboxylic acid, 7- β -D-glucopyranosyl-9,10-dihydro-3,5,6,8-tetrahydroxy-1-methyl-9,10-dioxo- **C86**
 9,10-anthracenedione **A220**
 9,10-anthracenedione, 2-amino- **A112**
 9,10-anthracenedione, 2-chloro- **C160**
 9,10-anthracenedione, 1,8-dihydroxy-3-(hydroxymethyl)- **A95**
 9,10-anthracenedione, 1,4,5,8-tetraamino- **C409**
 2-anthracylamine **A111**
 anthraflavic acid **A219**
 anthraflavin **A219**
 2-anthramine **A111**
 o-anthranilic acid **A115**
 anthranilic acid, cinnamyl ester **C347**
 anthraquinone **A220**
 9,10-anthraquinone **A220**
 anthraquinone, 2-chloro- **C160**
 α -anthraquinone, 1-chloro- **C159**
 1,5-anthraquinonediamine **D77**
 2,6-anthraquinonediamine **D78**
 anthraquinone, 1,4,5,8-tetramino- **C409**
 2-anthrylamine **A111**
 antibiotic FN 1636 **P92**
 antibiotic SF 767B **N38**
 Anticercospora **F26**
 Antideprin **I14**
 Antifoam FD62 **S32**
 Antigermina **P305**
 Antigram **M323**
 Antigram 95 GR **T226**
 Anti-Gro **C312**
 antihæmorrhagic vitamin **P181**
 antimalarina **M55**
 antimonate(2-), bis[μ -[2,3-dihydroxybutanedioato(4-)-O1,O2:O3,O4]]di-, dipotassium, trihydrate **A222**
 antimonie chloride **A223**
 antimonous chloride **A225**
 antimonous fluoride **A226**
 antimony **A221**
 antimony black **A221**
 antimony chloride **A223**
 antimony(III) chloride **A225**
 antimony(V) chloride **A223**
 antimony(III) fluoride **A226**
 antimony(V) fluoride **A224**
 antimonyl potassium tartrate **A222**
 antimonyl potassium tartrate hemihydrate **A222**
 antimony pentachloride **A223**
 antimony pentafluoride **A224**
 antimony perchloride **A223**
 antimony regulus **A221**
 antimony trichloride **A225**
 antimony trifluoride **A226**
 antimony trioxide **A227**
 antimony white **A227**
 antimycin A **A228**
 Antioxidant 116 **P124**
 antioxidant 4 **B245**
 antioxidant no. 33 **D155**
 antipellagra vitamin **N57**
 Antiperz **S97**
 Antirat **C238**
 antisal 2b **H101**
 Antiseptol **B51**
 Antisol 1 **T51**
 antisterility vitamin **T169**
 Antistrumin **P256**
 Antor **D282**
 Antoxol **D369**
 Antracine 12 **B244**
 Antracol **P307**
 antrapurol **D22**
 ANTU **N27**
 Antyperz **T226**
 ANU **A203**
 Anvil **H43**
 Anxiolit retard **O48**
 Anyvim **A209**
 Apache **C15**
 Apachlor **C128**
 apholate **A229**
 Aphoxide **T346**
 Aphrodine **Y1**
 Aphrosol **Y1**
 apiole **A230**
 Apistan **F94**
 Aplotin **D505**
 APO **T346**
 Apobas **B152**
 Apollo **C357**
 Appex **T60**
 Applaud **B194**
 Aprelazine **H85**
 Apresoline Hydrochloride **H85**
 AP-S **A183**
 aqua ammonia **A176**
 Aquacide **D560**
 aqua[[N,N'-1,2-ethanediylbis[(N-(carboxymethyl)-glycinato]]-(4-)-N,N',O,O',O'']cuprate(2-), disodium **C436**
 aqua fortis **N68**
 aqua mephyton **P181**
 Aquarius **H94**
 Aquathol **E22**

Aquisal **O46**
 1-(β-D-arabinofuranosyl)cytosine **C546**
 arabinosylcytosine **C546**
 arachic acid **E13**
 arachidic acid **E13**
 arachidonic acid **A231**
 Aragon **C448**
 aragran **T22**
 Araldite ERE 1359 **R6**
 Araldite hardener HY951 **T284**
 aramite **A232**
 Araton **A232**
 Arbax **L50**
 Arbochanchre **O50**
 Arbofog **D326**
 Arbuz **P3**
 arcanum duplicatum **P264**
 Arcillite **M349**
 Arcosolv DPM **D556**
 Arcton 6 **D204**
 Arcton 63 **T269**
 Arcton 7 **D216**
 Ardent **D327**
 areanum **P264**
 Arena **T14**
 Aresin **M345**
 Arezin **M345**
 Arezine **M345**
 Argenal **P118**
 argentium **S33**
 Argiflex **K2**
 Arlocardyl **P321**
 Arlytene **T155**
 Armeen O **O28**
 Armid E **E46**
 Armor **C545**
 Armoslip E **E46**
 Armyl **L66**
 Arnold's base **M212**
 Aroclor 1016 **A233**
 Aroclor 1221 **A234**
 Aroclor 1232 **A235**
 Aroclor 1242 **A236**
 Aroclor 1248 **A237**
 Aroclor 1254 **A238**
 Aroclor 1260 **A239**
 Aromabator PC-80 **C136**
 Aroquest 100 **E8**
 Arquad 16-29 **C105**
 Arrex **Z14**
 Arrex Toupeira **C41**
 arsanilic acid, monosodium salt **S43**
 Arsecodile **S63**
 Arsenal **I6**
 arsenic **A240**
 arsenic-75 **A240**
 arsenic acid **A241**

arsenic acid, calcium salt **C22**
 arsenic acid (H₃AsO₄), lead(2+) salt **L13**
 arsenic acid, lead salt **L13**
 arsenic acid, magnesium salt **M2**
 arsenic acid, sodium salt **S44**
 arsenicals **A240**
 arsenic black **A240**
 arsenic chloride **A243**
 arsenic(III) chloride **A243**
 arsenic dichloroethane **E112**
 arsenic disulfide **A242**
 arsenic hydride **A246**
 arsenic monosulfide **A242**
 arsenic oxide **A244**
 arsenic(III) oxide **A244**
 arsenic sesquioxide **A244**
 arsenic sesquisulfide **A245**
 arsenic sulfide **A245**
 arsenic sulfide **A242**
 arsenic sulfide red **A242**
 arsenic trichloride **A243**
 arsenic trihydride **A246**
 arsenic trioxide **A244**
 arsenic trisulfide **A245**
 arsenious acid **A244**
 arsenious acid, calcium salt **C23**
 arsenious acid, lead(2+) salt **L14**
 arsenious acid, sodium salt **S45**
 arsenious acid, trisilver(1+) salt **S34**
 arsenious chloride **A243**
 arsenious oxide **A244**
 arsenious sulfide **A245**
 arsenious trichloride **A243**
 arsenious trioxide **A244**
 arseniuretted hydrogen **A246**
 arsenous acid **A244**
 arsenous acid anhydride **A244**
 arsenous acid, potassium salt **P239**
 arsenous anhydride **A244**
 arsenous chloride **A243**
 arsenous hydride **A246**
 arsenous oxide **A244**
 arsenous oxide anhydride **A244**
 arsenous sulfide **A245**
 arsine **A246**
 arsine oxide hydroxydimethyl-, sodium salt **S63**
 arsine, thioxo- **A242**
 arsinic acid, dimethyl-, sodium salt **S63**
 arsonic acid, potassium salt **P239**
 arsonous dichloride, (2-chloroethenyl)- **L41**
 Artaban **B81**
 (6a*Rcis*)2,3,6a,9a-tetrahydro-4-methoxycyclopenta[c]furo-
 [3',2':4,5]furo[2,3-*h*][1]benzopyran-1,11-dione **A53**
 Arthrizon **P96**
 artificial ant oil **F120**
 artificial essential oil of almond **B40**
 Artisil Orange 3RP **A130**

Artosin **T171**
 Artrol **P300**
 Arvest **E63**
 Arvicolex **B152**
 Arvin **C63**
 Arylan CA **C32**
 AS **C98**
 Asalto **F21**
 Asana **E49**
 asbestos **A247**
 asbestos, white **C342**
 Ascabiol **B91**
 ascorbic acid **A248**
 Aseptia Brazilin **B27**
 Aseptameton **T134**
 Aseptia Oborex **C437**
 Aseptia Prebetox **E22**
 Aseptin A **E158**
 Asian Acid Orange EA **C390**
 Asian Acid Patent Blue VS 200% **C386**
 Asian Acid Red A **C397**
 Asian Acid Rhodamine B 400% **C396**
 Asian Direct Sky Blue FF **C405**
 asmacoril **F36**
 asphalt, fumes **A249**
 asphaltum **A249**
 Aspirin **A28**
 Aspon **T96**
 Assault **I6**
 Assert **I5**
 Assugrin **S59**
 astatine **A250**
 Astonex **D326**
 Astrix **M40**
 asulam **A251**
 Asuntol **C446**
 asymmetrical trimethylbenzene **T307**
 ATA **A158**
 atabrine **M55**
 atactic poly(vinyl chloride) **P235**
 Athado **T25**
 Athrombin **W3**
 Atlantic Black BD **C403**
 Atlas Somon **C145**
 atomic sulfur **S149**
 Atorel **I36**
 atrazine **A252**
 Atrinal **D362**
 atrochin **H122**
 atropine **A253**
 (-)-atropine **H124**
 A/T/S **E47**
 Attivar **Z19**
 Auger **I133**
 Aura **F20**
 auramine **A254**
 Aurantia **D550**

Aureomycin (as hydrochloride) **C316**
 auric chloride **G43**
 Aurora Yellow **C14**
 1-aurothio-D-glucopyranose **A255**
 aurothioglucose **A255**
 aurum paradoxum **T16**
 Australian gum **G53**
 Australol **I130**
 autigene MB **M60**
 automotive gasoline **G8**
 Avade **D69**
 Avadex BW **T198**
 Avantin **P297**
 Avenge **D325**
 Avgas **G8**
 aviation gasoline **G8**
 Avicel **C97**
 Avicol **Q12**
 Avlosulfon **S146**
 ayapanin **M133**
 10-azaanthracene **A34**
 5-aza-10-arsenaanthracene chloride **D541**
 azabenzene **P357**
 1-azacarbazole **C70**
 2-azacarbazole **C71**
 3-azacarbazole **C72**
 azaconazole **A256**
 azacycloheptane **H56**
 1-aza-2-cycloheptanone **C55**
 2-azacycloheptanone **C55**
 azacyclohexane **P201**
 1-aza-2,4-cyclopentadiene **P366**
 azacyclopentane **P367**
 azacyclopropane **A266**
 azacytidine **A257**
 5-azacytidine **A257**
 7-azadibenz[*a,h*]anthracene **D101**
 7-azadibenz[*a,j*]anthracene **D102**
 7-aza-7*H*-dibenzo[*c,g*]fluorene **D104**
 azadirachtin **A258**
 9-azafluorene **C64**
 1-azaindene **I31**
 2-azaindole **I22**
 azamethiphos **A259**
 1-azanaphthalene **Q9**
 2-azanaphthalene **I135**
 3-azapentane-1,5-diamine **D303**
 azaserin **A260**
 azaserine **A260**
 azathioprine **A261**
 Azařin **A258**
 1*H*-azepine-1-carbothioic acid, hexahydro-, *S*-ethyl ester
M337
 1-azetidinecarbonyl chloride **A262**
 Azidithion **M50**
 2-azido-4-(isopropylamino)-6-(methylthio)-*s*-triazine
A265

4-azido-4-isopropylamino-6-methylthio-1,3,5-triazine **A265**
 4-azido-*N*-(1-methylethyl)-6-methylthio-1,3,5-triazin-2-amine **A265**
 Aziflo **A264**
 Azimet **A264**
 azimethylene **D100**
 azimidobenzene **B78**
 Azimil **A264**
 Azin **A264**
 Azin **A263**
 3-azindole **B53**
 azine **P357**
 Azinfos **A263**
 Azinos **A263**
 azinphos-ethyl **A263**
 azinphos-methyl **A264**
 aziprotryn **A265**
 aziprotryne **A265**
 azirane **A266**
 aziridine **A266**
 aziridinylbenzoquinone **A267**
tris(1-aziridinyl)phosphine oxide **T346**
 1-aziridinylphosphonitrile trimer **A229**
 aziridyl benzoquinone **A267**
 aziridyl-*p*-benzoquinone **A267**
 azirino[2',3':3,4]pyrrolo[1,2-*a*]indole-4,7-dione, 6-amino-8-[[[(aminocarbonyl)oxy]methyl]-1,1a,2,8,8a,8b-hexahydro-8a-methoxy-5-methyl-, [1aS-(1α,8β,8α,8bα)]]- **M336**
 azirino [2',3':3,4]pyrrolo[1,2-*a*]indole-4,7-dione, 6-amino-1,1a,2,8,8a,8b-hexahydro-8-(hydroxymethyl)-8a-methoxy-5-methyl, carbamate(ester) **M336**
 Azobase DCA **D180**
 azobenzene **A268**
 azobenzene-2,4-diamine **D79**
 azobenzene oxide **A274**
 2-azobenzonitrile **C487**
 3-azobenzonitrile **C488**
 4-azobenzonitrile **C489**
 azobisbenzene **A268**
 azobiscarbonamide **A271**
 1,1-azobisformamide **A271**
 α,α'-azobisisobutyronitrile **A269**
 azobis(isobutyronitrile) **A269**
 2,2'-azobisisobutyronitrile **A269**
 azocyclotin **A270**
 azodibenzene **A268**
 azodibenzeneazofume **A268**
 azodicarbonamide **A271**
 azodicarboxamide **A271**
 azodicarboxylic acid diamide **A271**
 Azodrin **M343**
 Azodyne **P63**
 azoformamide **A271**
 Azogene Fast Blue B **D95**
 azoimide **H97**
 azol **A144**

azole **P366**
 azolmetazin **S133**
 Azomate **B81**
 azomycin **N124**
 azophenylene **P61**
 azoprocabazine **A272**
 Azopyrin **S140**
 azote **N119**
 azothoate **A273**
 Azotol A **N19**
 Azovan Blue **E190**
 azoxybenzene **A274**
 azoxybenzide **A274**
 azoxydibenzene **A274**
 Aztec CHP-80 **C475**
 Aztec TBHP-70, Aq **B261**
 Aztec TBPIB-75-OMS **B272**
 Azucaps **P74**
 Azulfidine **S140**
 B-1776 **T209**
 B500 **Q9**
 BA **D120**
 Ba 35846 **P185**
 Baciguent **B1**
 bacitracin **B1**
 Baigon **P315**
 Bakelite AYAA **P233**
 Bakelite DYNH **P224**
 bakelite LP80 **P231**
 bakelite QSAH **P235**
 BAL **D369**
 Bala **C543**
 Balfin **B29**
 Baltane **T247**
 Balwan **M343**
 Bamate **M57**
 Bamo **M57**
 banana oil **I80**
 Bancol **B37**
 Bandrowski's base **B2**
 banisterine **H7**
 Banocide **D295**
 BA (plasticiser) **D120**
 Barazen **Z17**
 barbaloin **B3**
 Barbamat **B4**
 barban **B4**
 Barbane **B4**
 Barbetol **C131**
 Barbidorm **H76**
 Barbital **P79**
 barbosec **Q3**
 Barclay Carbosect **C68**
 Barclay Desiquat **D560**
 Barclay Guideline **I133**
 Barclay Hurler **F88**
 Barclay Keeper **E72**

Barclay Winner **F39**
 Barhist **M118**
 barium **B5**
 barium acetate **B6**
 barium bromate **B7**
 barium bromide **B8**
 barium carbonate **B9**
 barium chlorate **B10**
 barium chloride **B11**
 barium cyanide **B12**
 barium diacetate **B6**
 barium dichloride **B11**
 barium dicyanide **B12**
 barium dinitrate **B13**
 barium dioxide **B17**
 barium disulfide **B18**
 barium monoxide **B14**
 barium nitrate **B13**
 barium oxide **B14**
 barium pentasulfide **B21**
 barium perchlorate **B15**
 barium permanganate **B16**
 barium peroxide **B17**
 barium polysulfides (BaS₂) **B18**
 barium polysulfides (Ba₂S₃) **B22**
 barium polysulfides (BaS₃) **B19**
 barium polysulfides (BaS₄) **B20**
 barium polysulfides (Ba₄S₇) **B23**
 barium polysulfides (BaS₅) **B21**
 barium protoxide **B14**
 barium sulfate **B24**
 barium superoxide **B17**
 barium tetrasulfide **B20**
 barium trisulfide (BaS₃) **B19**
 Barlay Dodex **D594**
 Barnon **F35**
 Baron **T261**
 Barosperse **B24**
 Barotrast **B24**
 Barseb HC **H95**
 Bartol **M32**
 baryta **B14**
 BAS 9021 **A71**
 Basagran **B38**
 Basev **C63**
 BAS 3170F **B31**
 BAS47900H **M98**
 basic cupric sulfate **B142**
 Basic Fuchsin **M1**
 Basic Green 1 **C400**
 Basic Orange 2 **C341**
 Basic Orange 3RN **C421**
 Basic Parafuchsin **C402**
 basic phenylmercuric nitrate **P120**
 Basic Red 1 **C401**
 Basic Red 9 **C402**
 Basic Rhodamine Yellow **C401**

Basic Violet 10 **R9**
 Basitac **M58**
 Basle Green **P15**
 Bassa **F12**
 Basta **G18**
 basudin **D99**
 Batalex **P305**
 Batasan **F25**
 battery manganese **M24**
 BAX **D538**
 BAY 21097 **O57**
 BAY 29952 **E150**
 BAY 37282 **T253**
 Bay 37344 **M123**
 BAY 38819 **P148**
 BAY 41831 **F11**
 Bay 68138 **F3**
 BAY 5712a **T191**
 Baycarb **F12**
 Baycid **F24**
 Baycor **B137**
 Baycoral **B137**
 BAY DRW1139 **M95**
 Bayer 38819 **P148**
 Bayer's acid **A135**
 Baygon **P315**
 Baygon MEB **P215**
 Bay-hox 1901 **E67**
 Baykor **B137**
 Bayluscid **N52**
 BAY NTN 9306 **S159**
 Baytan **T197**
 Baytex **F24**
 Baythion **P170**
 BBCE **I13**
 BBS **B142**
 BBSA **B248**
 BCM **M29**
 Beachklean **S74**
 BEAM **T272**
 Beesix **P359**
 Beetroot Red **B25**
 beet sugar **S131**
 Beflavin **R12**
 Befran **I10**
 Beldavrin **H123**
 Bellasol **B225**
 Belpron C **C59**
 Belsil CM 1000 **D373**
 Belt **C118**
 Belustine **L58**
 Benadon **P359**
 Benadryl **D537**
 Benadryl hydrochloride **D538**
 Benafine **B29**
 benalaxyl **B26**
 Benasalox **B27**

Benathion **M11**
 Benazalox **B27**
 benazolin **B27**
 benazoline **B27**
 Benazolinester **B27**
 bencarbate **B28**
 bendiocarb **B28**
 Bendopa **L37**
 Benecel **M185**
 Benefex **B29**
 Benex **B32**
 benfluralin **B29**
 Benfos **D258**
 benfuracarb **B30**
 Benfuracarbe **B30**
 Bengal isinglass **A58**
 Benicot **N53**
 Benlate **B32**
 Benocarb **C68**
 Benocten **D538**
 benodanil **B31**
 benomyl **B32**
 benorylate **B33**
 benoxaprofen **B34**
 benquinox **B35**
 bensulide **B36**
 bensultap **B37**
 Bensumec **B36**
 Bentazon **B38**
 bentazone **B38**
 benthiazole **T125**
 benthocarb **T117**
 Bentolite **M349**
 bentonite **B39**
 Bentopharm **B39**
 Bentrol **I59**
 Benural 70 **U12**
 Benylin **D537**
 Benzabar **T10**
 Benzac **T10**
 Benzac **B83**
 1,2-benzacenaphthene **F48**
 3,4-benz[*e*]acephenanthrylene **B56**
 Benzadone Golden Yellow **C428**
 benzahex **H9**
 benzal chloride **B98**
 benzaldehyde **B40**
 benzaldehyde, 3-chloro- **C162**
 benzaldehyde, *o*-chloro- **C161**
 benzaldehyde, 3,5-dibromo-4-hydroxy-, *O*-(2,4-dinitrophenyl)oxime **B176**
 Benzaldehyde Green **C400**
 benzalkonium chloride **B41**
 benzamide **B42**
 benzamide, *N,N*-diethyl-3-methyl- **D319**
 benzamidoacetic acid **H81**
 Benzamine Blue **T366**
 1,2-benzanthracene **B43**
 2,3-benzanthracene **N6**
 benz[*a*]anthracene **B43**
 benz[*b*]anthracene **N6**
 benzanthrene **B43**
 benzarone **B44**
 benzathine **B45**
 benzathine penicillin **B46**
 1-benzazine **Q9**
 2-benzazine **I135**
 benz-*o*-chlor **C164**
 benzenacetoneitrile **B97**
 benzenamine **A209**
 benzenamine, 4-[(4-aminophenyl)(4-imino-2,5-cyclohexadien-1-ylidene)methyl]-monohydrochloride **C402**
 benzenamine, 4-[(4-aminophenyl)(4-imino-3-methyl-2,5-cyclohexadien-1-ylidene)methyl]-2-methyl-, monohydrochloride **M1**
 benzenamine-*N*-butyl **B242**
 benzenamine, 4-chloro- **C156**
 benzenamine, 3-chloro-4-methoxy- **C158**
 benzenamine, 2,3-dichloro- **D178**
 benzenamine, 2,4-dichloro- **D179**
 benzenamine, 2,5-dichloro- **D180**
 benzenamine, 2,6-dichloro- **D181**
 benzenamine, 3,4-dichloro- **D182**
 benzenamine, *N,N*-diethyl- **D291**
 benzenamine, 4-(1,1-dimethylethyl)-*N*-(1-methylpropyl)-2,6-dinitro- **B232**
 benzenamine, 2-ethoxy- **P71**
 benzenamine hydrochloride **A210**
 benzenamine, 4-methoxy- **A215**
 benzenamine, 3-(trifluoromethyl)- **A118**
 benzenamine, 2,4,6-trinitro-*N*-2,4,6-trinitrophenyl **D550**
 benzenazobenzene **A268**
 benzene **B47**
 benzeneacetic acid, 4-chloro- α -(4-chlorophenyl) **B125**
 benzeneacetic acid, α -(hydroxymethyl)-8-methyl-8-azobicyclo[3.2.1]oct-3-yl ester *endo*-(\pm)- **A253**
 benzeneacetic acid, α -(hydroxymethyl)-, 9-methyl-3-oxa-9-azatricyclo [3.3.1.0^{2,4}]non-7-yl ester, hydrobromide, [7(*S*)-(1 α ,2 β ,4 β ,5 α ,7 β)- **H123**
 benzeneacetic acid, 2-propenyl ester **A91**
 benzeneacetyl chloride **P91**
 benzene aldehyde **B40**
 benzeneamine, 2,4-difluoro- **D329**
 benzeneamine, 4-(phenylazo)- **A114**
 benzenearsonic acid **P93**
 benzene azimide **B78**
 benzene-1-azo-2-naphthol **C426**
p-benzeneazophenol **C425**
 benzene, 1,4-bis[(chloromethoxy)methyl]- **B122**
 benzene, bromomethyl- **B92**
 benzene, 1-bromo-2-nitro- **B180**
 benzene, 1-bromo-4-nitro- **B181**
 benzene, 2-*tert*-butyl-1,4-dimethoxy- **B256**
 benzenecarbonyl **B40**

benzenecarbonyl chloride **B82**
 benzenecarboperoxoic acid, 1,1-dimethylethyl ester **B271**
 benzenecarboxylic acid **B63**
 1,2-benzenecarboxylic acid **P172**
 benzene chloride **C163**
 benzene, 1,1',1''-(1-chloro-1-ethenyl-2-ylidene)tris(4-methoxy)- **C299**
 1,2-benzenediamine **P102**
 1,3-benzenediamine **P101**
 1,4-benzenediamine **P103**
m-benzenediamine **P101**
 1,4-benzenediamine, 2,6-dichloro- **D240**
 1,3-benzenediamine dihydrochloride **P104**
 1,4-benzenediamine dihydrochloride **P105**
 1,3-benzenediamine, 4-(phenylazo)-, monohydrochloride **C341**
 benzene, dibromo- **D123**
 1,3-benzenedicarbonitrile **I114**
 1,3-benzenedicarbonitrile, 2,4,5,6-tetrachloro- **C286**
 1,2-benzenedicarboxamide **P171**
 1,2-benzenedicarboximide **P175**
 benzene-1,2-dicarboxylic acid **P172**
 1,4-benzenedicarboxylic acid **T26**
m-benzenedicarboxylic acid **I113**
p-benzenedicarboxylic acid **T26**
 1,2-benzenedicarboxylic acid anhydride **P173**
 1,2-benzenedicarboxylic acid, bis(2-butoxyethyl) ester **B116**
 1,2-benzenedicarboxylic acid, bis(2-methoxyethyl) ester **B130**
 1,2-benzenedicarboxylic acid, bis(2-methylpropyl) ester **D354**
 1,2-benzenedicarboxylic acid, butyl phenylmethyl ester **B94**
 1,2-benzenedicarboxylic acid, decyl octyl diester **O22**
 1,2-benzenedicarboxylic acid, dibutyl ester **D160**
 1,2-benzenedicarboxylic acid, dicyclohexyl ester **D268**
 1,2-benzenedicarboxylic acid, didecyl ester **D275**
 1,2-benzenedicarboxylic acid, didodecyl ester **D364**
 1,2-benzenedicarboxylic acid, diethyl ester **D314**
 1,2-benzenedicarboxylic acid, diheptyl ester **D340**
 1,2-benzenedicarboxylic acid, dihexyl ester **D341**
 1,2-benzenedicarboxylic acid, diisodecyl ester **D355**
 1,2-benzenedicarboxylic acid, dimethyl ester **D450**
 1,2-benzenedicarboxylic acid, dioctyl ester **D520**
 1,2-benzenedicarboxylic acid, dioctyl ester **D519**
 1,2-benzenedicarboxylic acid, di-2-propenyl ester **D72**
 1,2-benzenedicarboxylic acid, monobutyl ester **M341**
 1,2-benzenedicarboxylic acid, mono(2-ethylhexyl) ester **M344**
 1,2-benzenedicarboxylic acid, monoethyl ester **M346**
 1,2-benzenedicarboxylic acid, monopentyl ester **M347**
 benzene, 1,3-dichloro-5-methoxy- **D186**
 benzene, 1,2-dichloro-4-nitro- **D230**
 benzene, 1,2-diethyl- **D292**
 benzene, 1,3-diethyl- **D293**
 benzene, 1,4-diethyl- **D294**
 benzene, *p*-diethyl- **D294**
 benzene, 1,4-diisothiocyanato- **B138**
 1,3-benzenedimethanamine **X17**
 benzene, 2-(1,1-dimethylethyl)-1,4-dimethoxy- **B256**
 benzene, 1,1-(1,1-dimethylethyl)-4-methyl **B278**
 1,2-benzenediol **C95**
 1,3-benzenediol **R5**
 1,4-benzenediol **H107**
o-benzenediol **C95**
p-benzenediol **H107**
 1,4-benzenediol, 2-(1,1-dimethylethyl)- **B262**
 benzenethanol **P67**
 benzenethanol, 4-chloro-β-(4-chlorophenyl)- **B126**
 benzenethanol, α-[2-(dimethylamino)-1-methylethyl]-α-phenyl-, propanoate (ester), [R-(R'S')] **L39**
 benzenethanol, α-[2-(dimethylamino)-1-methylethyl]-α-phenyl-, propanoate (ester), hydrochloride, [S-(R*,S*)]- **P319**
 benzene hexachloride **H9**
 ε-benzene hexachloride **L48**
 γ-benzene hexachloride **H10**
 benzene iodide **I45**
 benzene, iodo- **I45**
 benzene, (2-isothiocyanatoethyl)- **P70**
 benzenemethanamine **B90**
 benzenemethanamine, *N*-(2-chloroethyl)-*N*-(1-methyl-2-phenoxyethyl)-, hydrochloride **P85**
 Benzenemethanaminium, *N*-[4-[[4-(dimethylamino)phenyl][4-[ethyl[(3-sulfofophenyl)methyl]amino]phenyl]methylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-3-sulfo-, hydroxide, inner salt, sodium salt **B101**
 benzenemethanaminium *N,N*-dimethyl *N*-[2-[2-[4-[1,1,3,3-tetramethylbutyl]phenoxy]ethoxy]ethyl]chloride **B51**
 benzenemethanaminium, *N*-ethyl-*N*-[4-[[4-[ethyl[(3-sulfofophenyl)methyl]amino]phenyl](2-sulfofophenyl)methylene]-2,5-cyclohexadien-1-ylidene]-3-sulfo inner salt, diammonium salt **C387**
 benzenemethanol **B89**
 benzenemethanol, 4-chloro-α-(4-chlorophenyl)-α methyl- **C125**
 benzenenitrile **B68**
p-benzenenitrile **T27**
 benzenepropanal, 4-(1,1-dimethylethyl)-α-methyl- **L44**
 benzenepropanamine, *N*-methyl-γ-[4-(trifluoromethyl)phenoxy]-, hydrochloride, (±)- **F82**
 benzenepropanaminium bromide **E16**
 benzenesulfochloride **B48**
 benzene sulfohydrazide **B49**
 benzenesulfonamide, 4-acetyl-*N*-[(cyclohexylamino)carbonyl] **A15**
 benzenesulfonamide, 4-chloro-*N*-[(propylamino)carbonyl]- **C311**
 benzenesulfochloride **B48**
 benzenesulfonic acid, 2-amino **A211**
 benzenesulfonic (acid) chloride **B48**
 benzenesulfonic acid, 4-chlorophenyl ester **F22**

- benzenesulfonic acid, dodecyl-, calcium salt **C32**
benzenesulfonic acid, dodecyl-, sodium salt **S65**
benzenesulfonic acid, 4-[(2-hydroxy-1-naphthalenyl)azo]-, monosodium salt **C391**
benzenesulfonic acid, thio-*S,S'*-(2-(dimethylamino)trimethylene)ester **B37**
benzenesulfonyl chloride **B48**
benzenesulfonyl hydrazide **B49**
1,2,4,5-benzenetetracarboxylic 1,2:4,5-dianhydride **P364**
benzene, tetrachloronitro- **T14**
benzenetetrahydride **C511**
benzenethanamine **P69**
benzenethiol **B50**
1,2,4-benzenetricarboxylic acid anhydride **T299**
benzene, 1,3,5-trimethyl- **M90**
1,2,3-benzenetriol **P363**
benzenol **P80**
benzenyl fluoride **B80**
benzenyltrichloride **B79**
benzethonium chloride **B51**
2,3-benzofluoranthene **B56**
3,4-benzofluoranthene **B56**
benz[*j*]fluoranthene **B58**
(*N*-benzhydryl)(*N'*-methyl)diethylenediamine **C497**
N-benzhydryl-*N'*-methylpiperazine **C497**
2-(benzhydryloxy)-*N,N*-dimethylethylamine **D537**
benzidine **B52**
benzidine, 3,3'-dimethoxy- **D95**
benzidine yellow **D96**
Benzilan **C164**
benzimidazole **B53**
2-benzimidazolecarbamic acid, methyl ester **C65**
2-benzimidazolethiol **M60**
4-(2-benzimidazolyl)thiazole **T111**
benziminazole **B53**
benzin **G8**
Benzin B70 **N5**
1,2-benzisothiazolin-3-one **B54**
1,2-benzisothiazolin-3(2*H*)-one 1,1-dioxide **S1**
1,2-benzisothiazol-3(2*H*)-one **B54**
benzocaine **B55**
1*H*,3*H*-benzo(1,2-*c*,4,5-*c'*)difuran-1,3,5,7-tetrone **P364**
benzochinamide **B62**
benzo[*d,e,f*]chrysene **B71**
benzocyclohexane **T80**
benzocyclopentane **I17**
4*H*-1,3,2-benzodioxaphosphorin, 2-methoxy-, 2-sulfide **D527**
1,3-benzodioxol-4-ol, 2,2-dimethyl-, methylcarbamate **B28**
(*E,E*)-1-[5-(1,3-benzodioxol-5-yl)-1-oxo-2,4-pentadienyl]piperidine **P203**
β-benzoepin **E20**
benzoepin sulfate **E21**
5,6-benzoflavone **N14**
7,8-benzoflavone **N13**
benzo(1)fluoranthene **B58**
10,11-benzofluoranthene **B58**
11,12-benzofluoranthene **B59**
2,13-benzofluoranthene **B57**
7,10-benzofluoranthene **B57**
7,8-benzofluoranthene **B58**
8,9-benzofluoranthene **B59**
benzo[*b*]fluoranthene **B56**
benzo[*e*]fluoranthene **B56**
benzo[*ghi*]fluoranthene **B57**
benzo[*j*]fluoranthene **B58**
benzo[*k*]fluoranthene **B59**
benzo[*mno*]fluoranthene **B57**
1,2-benzofluorene **B60**
11*H*-benzo[*a*]fluorene **B60**
benzo[*a*]fluorene **B60**
benzo[*jk*]fluorene **F48**
benzofos **P149**
benzofuran **B61**
2,3-benzofuran **B61**
benzo[*b*]furan **B61**
3-benzofurancarboxylic acid, 2-(2,4-dihydroxyphenyl)-6-hydroxy-, δ-lactone **C449**
7-benzofuranol, 2,3-dihydro-2,2-dimethyl-, methylcarbamate **C68**
2(4*H*)-benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (*R*)- **D342**
benzofurfuran **B61**
6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, 3,9-dihydroxy- **C449**
benzoglyoxaline **B53**
benzoguanamine **B62**
benzoic acid **B63**
benzoic acid amide **B42**
benzoic acid, ammonium salt **A164**
benzoic acid benzyl ester **B91**
benzoic acid, *p*-*tert*-butyl **B249**
benzoic acid chloride **B82**
benzoic acid, 5-[[4'-[[2,6-dihydroxy-3-[(2-hydroxy-5-sulphophenyl)azo][1,1'-biphenyl]-4-yl]azo]-2-hydroxy-, copper complex **C407**
benzoic acid, 4-(1,1-dimethylethyl) **B249**
benzoic acid, *o*-[6-(ethylamino)-3-(ethylimino)-2,7-dimethyl-3*H*-xanthen-9-yl]-, ethyl ester, monohydrochloride **C401**
benzoic acid ethyl ester **E99**
benzoic acid, 4-hydroxy-, butyl ester **B269**
benzoic acid [4-hydroxyimino)-2,5-cyclohexadien-1-ylidene]hydrazide **B35**
benzoic acid, 2-iodyl-, calcium salt **C35**
benzoic acid, 2-[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonylamino]sulfonyl]-, methyl ester **M328**
benzoic acid methyl ester **M161**
benzoic acid nitrile **B68**
benzoic acid, phenyl ester **P94**
benzoic acid phenylmethyl ester **B91**
benzoic acid, 3,4,5-trihydroxypropyl ester **P332**
benzoic ether **E99**

benzoic trichloride **B79**
 benzoimidazole **B53**
 benzoin **B64**
 4,5-benzoindotricarbocyanine **I30**
 benzoisothiazolin-3-one **B54**
 benzol **B47**
 160° Benzol **N5**
 benzole **B47**
 Benzo Leather Black E **C403**
 benzo[l]phenanthrene **T336**
 Benzomate **B81**
 benzo[b]naphtho[1,2-*d*]thiophene **B65**
 benzo[b]naphtho[2,1-*d*]thiophene **B66**
 benzo[b]naphtho[2,3-*d*]thiophene **B67**
 benzonitrile **B68**
 benzo[*rst*]pentaphene **D117**
 1,12-benzoperylene **B69**
 benzo[*ghi*]perylene **B69**
 1,2-benzophenanthrene **C340**
 9,10-benzophenanthrene **T336**
 benzo[*a*]phenanthrene **C340**
 benzo[*def*]phenanthrene **P351**
 benzophenone **B70**
 benzophenone-1 **B85**
 benzophenone 6 **D349**
 benzophosphate **P149**
 [1]benzopyrano[3,4-*b*]furo[2,3-*h*][1]benzopyran-6 (6*aH*)-one, 1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-, [2*R*-(2*α*,6*α*,12*α*)]- **R18**
 2*H*-1-benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, [2*R*-(4*R**,8*R**)]]- **T169**
 2*H*-1-benzopyran-2-one **C447**
 4*H*-1-benzopyran-4-one, 3-[[6-*O*-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- **R22**
 4*H*-1-benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)- **G9**
 4*H*-1-benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-7-hydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one **D18**
 1*H*-benzopyrazole **I22**
 3,4-benzopyrene **B71**
 6,7-benzopyrene **B71**
 benzo[*a*]pyrene **B71**
 benzo[*e*]pyrene **B72**
 benzopyridine **Q9**
 benzopyridine **I135**
 benzo[*c*]pyridine **I135**
 1,2-benzopyrone **C447**
 1-benzo- α -pyrone **C447**
 2,3-benzopyrrole **I31**
 2,3-benzoquinoline **A34**
 benzo(*b*)quinoline **A34**
 1,2-benzoquinone **B73**
 1,4-benzoquinone **B74**
 2-benzoquinone **B73**
 4-benzoquinone **B74**
o-benzoquinone **B73**
p-benzoquinone **B74**
 benzoquinone aziridine **A267**
 1,4-Benzoquinone-*N'*-benzoylhydrazone oxime **B35**
 1,4-benzoquinone dioxime **B75**
p-benzoquinone dioxime **B75**
p-benzoquinone monophenylhydrazone **C425**
 Benzoresorcinol **B85**
 benzosulfimide **S1**
 benzosulfonazole **B76**
 benzosulfonic acid, zinc salt (2:1) **Z13**
 3,4-benzo-9-thiafluorene **B65**
 benzothiazole **B76**
 benzothiazole disulfide **D572**
 2-benzothiazolethiol **M61**
 2(3*H*)-benzothiazolethione, zinc salt **Z10**
 1-benzothiazol-2-yl-1,3-dimethylurea **M101**
 1-(1,3-benzothiazol-2-yl)-1,3-dimethylurea **M101**
 1-(2-benzothiazolyl)-1,3-dimethylurea **M101**
N-2-benzothiazolyl-*N'*-dimethylurea **M101**
 2-benzothiazol-2-yloxy-*N*-methylacetanilide **M41**
 2-(2-benzothiazolylloxy)-*N*-methyl-*N*-phenyl acetamide **M41**
 1-(2-benzothiazolyl)-3-methylurea **B87**
 benzothiofuran **B77**
 1-benzothiophene **B77**
 benzo[*b*]thiophene **B77**
 benzo[*c*]thiophene, 1,3-dihydro- **D343**
 benzotriazole **B78**
 1*H*-benzotriazole **B78**
 benzotrichloride **B79**
 benzotrifluoride **B80**
 benzoximate **B81**
 benzoyl amide **B42**
 benzoylamidoacetic acid **H81**
 benzoylbenzene **B70**
 benzoyl *tert*-butylperoxide **B271**
 benzoyl chloride **B82**
 benzoyl cyanide-*o*-(diethoxy phosphinothioyl)oxime **P170**
N-benzoyl-*N*-(3,4-dichlorophenyl)-L-alanine ethyl ester **B84**
 benzoylglycine **H81**
N-benzoylglycine **H81**
m-benzoylhydratopic acid **K10**
 3-benzoylhydratopic acid **K10**
 4-benzoyl-hydrazona-1,4-benzoquinone oxime **B35**
 benzoyl methide **A21**
 3-benzoyl- α -methylbenzeneacetic acid **K10**
 (benzoyloxy)tributylstannane **T214**
 benzoyl peroxide **B83**
 benzoylphenylcarbinol **B64**
 benzoylprop-ethyl **B84**
 4-benzoylresorcinol **B85**
 benzoyl superoxide **B83**
 α -benzoyltriethylamine **D315**
 1,12-benzperylene **B69**
 2,3-benzphenanthrene **B43**

benzphetamine **B86**
 1,2-benzpyrene **B72**
 3,4-benzpyrene **B71**
 4,5-benzpyrene **B72**
 benz[a]pyrene **B71**
 benzoquinamide **B62**
 1*H*-2,1,3-benzthiadiazin-4(3*H*)-one, 3-isopropyl-2,2-dioxide-
B38
 benzthiazuron **B87**
 benzyl acetate **B88**
 benzyl alcohol **B89**
 benzylamine **B90**
 benzylamine, *N*-(2-chloroethyl)-*N*-(1-methyl-2-
 phenoxyethyl)-, hydrochloride **P85**
 benzylbenzene **D547**
 benzylbenzenecarboxylate **B91**
 benzyl benzoate **B91**
 benzyl bromide **B92**
 benzyl bromoacetate **B93**
 benzyl butyl phthalate **B94**
N'-[(2-benzylcarbamoyl)ethyl]isonicotinoylhydrazide
N43
 benzyl carbinol **P67**
 benzylcarbonyl acetate **P66**
 benzyl chloride **B95**
 2-benzyl-4-chlorophenol **B96**
o-benzyl-*p*-chlorophenol **B96**
 benzyl cyanide **B97**
 benzyl dichloride **B98**
 benzyldimethylalkyl(C₁₄-C₁₆)ammonium chloride **A66**
 benzyldimethylamine **D403**
N-benzyl-*N*, α -dimethylphenethylamine **B86**
S-benzyl dipropylthiocarbamate **P340**
 benzylene chloride **B98**
 benzyl ethanoate **B88**
 benzyl ether **D120**
 benzylhexadecyldimethylammonium chloride **C103**
 benzylidene chloride **B98**
 benzylidene fluoride **B80**
 benzyl isoeugenol **B99**
 benzyl isoeugenol ether **B99**
N-benzyl- β -(isonicotinoylhydrazino)propionamide **N43**
 α -benzylisopropylamine **P88**
 benzyl 2-methoxy-4-propenylphenyl ether **B99**
 benzyl methyl ether **M166**
 benzyl oxide **D120**
 benzylpenicillin **B100**
 benzylpenicillanic acid **B100**
 5-benzyl-2,3,4,5-tetrahydro-2-methyl-1*H*-pyrido[4,3-
 b]indole **M36**
 benzyl trichloride **B79**
 Benzyl Violet 3B **B101**
 Benzyl Violet 4B **B101**
 B(e)P **B72**
 Berkfurin **N115**
 Berkomine **I15**
 Berol 370 **P218**

Beronald **F112**
 Berthallet salt **P242**
 Berubigen **C368**
 beryllium **B102**
 beryllium chloride **B103**
 beryllium dichloride **B103**
 beryllium difluoride **B104**
 beryllium fluoride **B104**
 beryllium nitrate **B105**
 beryllium sulfate **B106**
 Beskor **E40**
 Best Acid Brilliant Blue EA New **C387**
 Best Acid Rhodamine FB 400% **C396**
 Betalin 12 Crystalline **C368**
 Betamin **C131**
 Betanal **P78**
 betanex **D59**
 betanin **B107**
 Betaprone **P308**
 Betasan **B36**
 Betatab **C89**
 Better **C131**
 betula oil **M305**
 Bexone **M34**
 bezatin **P358**
 B(*b*)F **B56**
 BHA **B244**
 BHC **H9**
 ϵ -BHC **L48**
 γ -BHC **H10**
 BHT **B245**
 BI-5452 **F15**
 Bi 58 **D376**
 BZI **B53**
 4',4''-biacetanilide **D67**
 biacetyl **B209**
N,N'-bianiline **D546**
o,p'-bianiline **D543**
p,p'-bianiline **B52**
 bibenzal **S115**
 bibenzylidene **S115**
 BIC **B264**
cis-bicyclo[4.4.0]decane **D38**
 bicyclo[2.2.1]hepta-2,5-diene **N202**
 bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-*endo*- **B143**
 bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (\pm) **C53**
 bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl- **C50**
 bicyclo[2.2.1]hept-2-ene **V34**
 bicyclopentadiene **D271**
 Bideron **P341**
 Bidiphen **T122**
 Bidisin **C126**
 Bidrin **D263**
 bifenox **B108**
 bifenthrin **B109**
 Biflex **B109**
 biformyl **G39**

biformylchlorazin **T295**
 biisobutenyl **D419**
 biisocrotyl **D419**
 Bikartol **P305**
 bilanafos **B110**
 bimethyl **E58**
 Binafos **C128**
 binapacryl **B111**
 2,3,1'8'-binaphthylene **B59**
 Bioban GK **H51**
 Bio-Beads **D580**
 biocarbazine R **D17**
 Bio-DES **S116**
 Biofanal **N210**
 Biokill **P56**
 Biokor **N22**
 BioMeT 204 **T341**
 biomet TBTO **T219**
 Bio Neem **A258**
 Biopar Forte **C368**
 Biophedrin **E30**
 Bioquin **H119**
 Bio Racumin **C448**
 Biosterol **R7**
 Bio Strike **C59**
 Biothion **T19**
 biotin **B112**
d-(+)-biotin **B112**
 bioxin **V17**
 bioxirane **D278**
 2,2'-bioxirane **D278**
 (*R**,*R**)-(±)-2,2'-bioxirane **D279**
 (*R**,*S**)-2,2'-bioxirane **D280**
 bioxone **M120**
 biphenyl **B113**
 biphenyl-4-amine **A121**
 (1,1'-biphenyl)-2-amine **A121**
 (1,1'-biphenyl)-2-amine **A119**
 (1,1'-biphenyl)-3-amine **A120**
 2-biphenylamine **A119**
 3-biphenylamine **A120**
 4-biphenylamine **A121**
o-biphenylamine **A119**
p-biphenylamine **A121**
 (1,1'-biphenyl)-2,4-diamine **D543**
 [1,1'-biphenyl]-4,4'-diamine **B52**
 2,4'-biphenyldiamine **D543**
 1,1'-biphenyl-4,4'-diamine, 2,2'-dichloro- **D191**
 [1,1'-biphenyl]-4,4'-diamine, 3,3'-dimethoxy- **D95**
 2,5-biphenyldiol **P110**
N,N'-(1,1'-biphenyl)-4,4'-diylbisacetamide **D67**
 (1,1'-biphenyl)-2,2'-diyl oxide **D111**
 biphenyl-4,4'-enediamine **B52**
o-biphenylenemethane **F49**
 2,2'-biphenylene oxide **D111**
 biphenylmethane **D547**
 [1,1'-biphenyl]-2-ol **P125**
 [1,1'-biphenyl]-3-ol **P126**
 [1,1'-biphenyl]-4-ol **P127**
 2-biphenylol **P125**
 4-biphenylol **P127**
m-biphenylol **P126**
 2-biphenylol, sodium salt **S86**
 biphenyl oxide **D544**
 (1,1'-biphenyl-4-yl)acetamide **P90**
N,N'-4,4'-biphenylenebisacetamide **D67**
 β-[(1,1'-biphenyl)-4-yloxy]-α-(1-1-dimethylethyl)-1*H*-1,2,4-triazole-1-ethanol **B137**
 (1*RS*,2*RS*:1*RS*,2*SR*)-1-biphenyl-4-yloxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)butanol-2-ol [20:80 ratio of (1*RS*,2*RS* and (1*RS*,2*SR*) isomers **B137**
 3-(3-[1,1'-biphenyl]-4-yl)-1,2,3,4-tetrahydro-1-naphthalenyl)-4-hydroxy-2*H*-1-benzopyran-2-one **D323**
 3-(3-[1,1'-biphenyl-4-yl]-1,2,3,4-tetrahydro-1-naphthyl)-4-hydroxycoumarin **D323**
 bipotassium chromate **P244**
 Birgin **P305**
 Birgin **C312**
 Birlane **C128**
 bis(acetato)dihydroxytrilead **L29**
 bis(acetato-*O*)dioxo-uranium **U10**
 bis(acetoxy)cadmium **C3**
 2,2'-bis(acryloyloxymethyl)butyl acrylate **T311**
 Bisamine S **M210**
 bis(4-amino-3-chlorophenyl) ether **O54**
 bis(4-amino-3-chlorophenyl)methane **M210**
 bis(4-aminocyclohexyl)methane **D272**
 bis(*p*-aminocyclohexyl)methane **D272**
 bis(2-aminoethyl)amine **D303**
N,N'-bis(2-aminoethyl)-1,2-ethanediamine **T284**
 4,4'-bis[7-(1-amino-8-hydroxy-2,4-disulfo)naphthylazo]-3,3'-bitolyl, tetrasodium salt **E190**
 bis(*p*-aminophenyl) ether **O58**
 2',4-bis(aminophenyl)methane **M217**
 bis(4-aminophenyl)methane **M218**
 bis(*p*-aminophenyl) sulfide **T127**
 bis(4-aminophenyl)sulfone **S146**
N,N'-bis(3-aminopropyl)-1,4-butanediamine **S107**
 2,5-bis(1-aziridinyl)-3,6-bis(2-methoxyethoxy)-1,4-benzoquinone **A267**
 2,5-bis(1-aziridinyl)-3,6-bis(2-methoxyethoxy)-2,5-cyclohexadiene-1,4-dione **A267**
 1,2-bis(benzylamino)ethane **B45**
 bis[bisdimethyl aminophosphorus] anhydride **S9**
 1,4-bis(bromoacetoxy)-2-butene **B114**
 2,2-bis(bromomethyl)-1,3-propanediol **D134**
 bis(4-bromophenyl) ether **B115**
 5-[bis[2-(2-butoxyethoxy)ethoxy]methyl]-1,3-benzodioxole **P207**
 1,1-bis[2-(2-butoxyethoxy)ethoxy]methyl-3,4-methylenedioxybenzene **P207**
 bis(2-butoxyethyl) phthalate **B116**
 1,1-bis(*tert*-butyldioxy)-3,3,5-trimethylcyclohexane **B117**
 bis(2-*tert*-butyl-4-hydroxy-6-methylphenyl)sulfide **T118**

1,1-bis(*tert*-butylperoxy)-3,3,5-trimethylcyclohexane **B117**
 2,4-bis(*tert*-butyl)phenol **D155**
 1,3-bis(carbamoylthio)-2-(*N,N*-dimethylamino)propane hydrochloride **C92**
N,N-bis(carboxymethyl)glycine **N70**
N,N-bis(carboxymethyl)glycine trisodium salt monohydrate **T358**
 bis(3-carboxypropionyl) peroxide **D564**
 bis(4-chlorobenzoyl) peroxide **C171**
 bis(2-chloroethoxy)methane **B118**
 4-[bis(2-chloroethyl)amino]benzenebutanoic acid **C111**
 1,6-bis(2-chloroethylamino)-1,6-dideoxy-D-mannitol dihydrochloride **M29**
 2-(bis(2-chloroethyl)amino)-1-oxa-3-aza-2-phosphacyclohexane 2-oxide **C529**
 4-[bis(2-chloroethyl)amino]-L-phenylalanine **M49**
 DL-3-[[*p*-bis(2-chloroethyl)amino]phenyl]alanine **M88**
 4-[*p*-[bis(2-chloroethyl)amino]phenyl]butyric acid **C111**
N,N-bis(β-chloroethyl)amino-*N'*-*O*-propylenephosphoric acid ester diamide **I3**
 5-(bis(2-chloroethyl)amino)-2,4(1*H*,3*H*)pyrimidinedione **B119**
 5-bis(2-chloroethyl)aminouracil **B119**
 5-*N,N*-bis(2-chloroethyl)-aminouracil **B119**
 bis(2-chloroethyl) ether **B120**
 bis(β-chloroethyl) ether **B120**
 bis(2-chloroethyl)ethylamine **H82**
 bis(β-chloroethyl)formal **B118**
 bis(2-chloroethyl)methylamine **M38**
 bis(β-chloroethyl)methylamine **M38**
N,N-bis(2-chloroethyl)-2-naphthylamine **C142**
 1,3-bis(chloroethyl)-1-nitrosourea **B121**
 1,3-bis(β-chloroethyl)-1-nitrosourea **B121**
 bis(β-chloroethyl) sulfide **M359**
N,3-bis(2-chloroethyl)tetrahydro-2*H*-1,3,2-oxazaphosphorin-2-amine, 2-oxide **I3**
 bis(chlorohydroxyphenyl)methane **D235**
 bis(β-chloroisopropyl) ether **D221**
 1,4-bis(chloromethoxymethyl)benzene **B122**
 bis-1,4-(chloromethoxy)-*p*-xylene **B122**
 bis(chloromethyl) ether **B123**
 bis(2-chloro-1-methylthyl) ether **D26**
 bis(chloromethyl)ketone **D174**
 3,3-bis(chloromethyl)oxetane **B124**
 bis(4-chlorophenyl)acetic acid **B125**
 1,1-bis(*p*-chlorophenyl)-2-chloroethane **D32**
 1,1-bis(*p*-chlorophenyl)-2-chloroethylene **D33**
 2,2-bis(4-chlorophenyl)-1,1-dichloroethane **D30**
 2,2-bis(4-chlorophenyl)-1,1-dichloroethylene **D31**
N,N'-bis(4-chlorophenyl)-3,12-diimino-2,4,11,13-tetraazatetradecanediimidamide **C130**
 1,1-bis(4-chlorophenyl)ethanol **C125**
 2,2-bis(4-chlorophenyl)ethanol **B126**
 2,2-bis(*p*-chlorophenyl)ethanol **B126**
 1,2-bis(2-chlorophenyl)hydrazine **D218**
 2,2-bis(4-chlorophenyl)-1-hydroxyethane **B126**
 bis(4-chlorophenyl) sulfone **B127**

3,6-bis(2-chlorophenyl)-1,2,4,5-tetrazine **C357**
 1,1'-bis(4-chlorophenyl)-2,2,2-trichloroethane **D35**
 2,2-bis(*o,p'*-chlorophenyl)-1,1,1-trichloroethane **D34**
 1,1-bis(*p*-chlorophenyl)-2,2,2-trichloroethanol **D261**
N,N'-bis[4-chloro-3-(trifluoromethyl)phenyl]urea **F42**
 bis(*p*-chlorophenyl)acetic acid **B125**
 Biscomate **B138**
 bis(cyanoethyl)amine **I13**
 bis(cyclohexyl)carbodiimide **D267**
 1,3-bis(cyclohexyl)thiourea **D269**
 biscyclopentadiene **D271**
 bis(cyclopentadienyl)iron **F32**
 2,2-bis(3,5-dibromo-4-hydroxyphenyl)propane **T39**
 bis(diethyldithiocarbamate)zinc **Z9**
 bis-*O,O*-diethylphosphoric anhydride **T68**
 bis(diethylthiocarbamoyl)disulfide **D565**
 bis(2,4-dihydroxyphenyl)methanone **T78**
 bis(dimethylamido)fluorophosphate **D367**
p-bis(dimethylamine)benzene **T92**
 3,6-bis(dimethylamino)acridine **C421**
 bis(dimethylamino)-3-amino-5-phenyltriazolyl phosphine oxide **T202**
 4,4'-bis(dimethylamino)benzophenone **B128**
p,p'-bis(*N,N*-dimethylamino)benzophenone **B128**
 4,4-bisdimethylaminobenzophenoneimide **A254**
 1,2-bis(dimethylamino)ethane **T89**
 3,7-bis(dimethylamino)phenothiazin-5-ium chloride **M216**
 bis-[4-(dimethylamino)phenyl]methanone **B128**
 bis(*p*-dimethylaminophenyl)methyleneimine **A254**
 bis[*p*-(dimethylamino)-phenyl]phenylmethylium chloride **M9**
 bis(α,α-dimethylbenzyl) peroxide **D264**
 (*T*₄)-bis(dimethyldithiocarbamate-*S,S'*)zinc **Z19**
 bis(dimethyldithiocarbamate)lead **L18**
 3,5-bis(1,1-dimethylethyl)-4-hydroxybenzoic acid **D148**
 2,6-bis(1,1-dimethylethyl)-4-methylphenol **B245**
 bis(1,1-dimethylethyl) peroxide **D150**
 2,4-bis(1,1-dimethylethyl)phenol **D155**
 2,6-bis(1,1-dimethylethyl)phenol **D156**
 3,5-bis(1,1-dimethylethyl)phenol **D157**
 bis(dimethylthiocarbamoyl) disulfide **T147**
 bis(dimethylthiocarbamoyl) sulfide **M348**
 bis(*O,O*-dipropyl) phosphorothionic anhydride **T96**
 Bisecurin I **O41**
 1,3-bis(2,3-epoxypropoxy)benzene **R6**
m-bis(2,3-epoxypropoxy)benzene **R6**
 1,4-bis(2,3-epoxypropoxy)butane **B208**
 1,2-bis(2,3-epoxypropoxy)ethane **E118**
 1,2-bis[2-(2,3-epoxypropoxy)ethoxy]ethane **T282**
 bis(2,3-epoxypropyl)aniline **D336**
N,N-bis(2,3-epoxypropyl)aniline **D336**
 bis(2,3-epoxypropyl) ether **D337**
 bis(epoxypropyl)phenylamine **D336**
 bis(1,2-ethanediamine-*N,N'*-copper(II)) **C477**
S-[1,2-bis(ethoxycarbonyl)ethyl] *O,O*-dimethyl phosphorodithioate **M11**

bis(2-ethoxyethyl) ether **E80**
 2,4-bis(ethylamino)-6-methylthio-1,3,5-triazine **S38**
 2,4-bis(ethylamino)-6-(methylthio)-s-triazine **S38**
 1,1'-bis(ethylene oxide) **D278**
 bis(2-ethylhexyl) adipate **D514**
 bis(2-ethylhexyl)amine **D515**
 1,3-bis(2-ethylhexyl)hexahydro-5-methyl-5-pyrimidinamine **H75**
 bis(2-ethylhexyl) hydrogen phosphate **D518**
 bis(2-ethylhexyl)orthophosphoric acid **D518**
 bis(ethylhexyl) peroxydicarbonate **D517**
 bis(2-ethylhexyl) peroxydicarbonate **D517**
 bis(2-ethylhexyl) phosphate **D518**
 bis(2-ethylhexyl) phthalate **D519**
 1,4-bis(2-ethylhexyl) sulfobutanedioate **D583**
 bis(2-ethylhexyl) sulfosuccinate **D583**
 bisethylxanthogen **D582**
 bisethylxanthogen sulfide **D582**
 1-[[bis(4-fluorophenyl)methylsilyl]-methyl]-1*H*-1,2,4-triazole **F90**
 bis(4-fluorophenyl)methyl (1*H*-1,2,4-triazol-1-ylmethyl)-silane **F90**
 1,2-bis(glycidylloxy)ethane **E118**
 bis(2-hexyloxyethyl) adipate **B129**
 bis[2-hydroxy-5-chlorophenyl] sulfide **T121**
 bishydroxycoumarin **D262**
 bis(2-hydroxyethyl)amine **D281**
 bis(2-hydroxyethyl)carbamidithioic acid, monopotassium salt **P240**
N,N-bis(hydroxyethyl)-coco-amides **C381**
 bis(2-hydroxyethyl)dithiocarbamic acid, monopotassium salt **P240**
 bis(2-hydroxyethyl)dithiocarbamic acid, potassium salt **P240**
N,N-bis(2-hydroxyethyl)dodecanamide **L7**
 bis(2-hydroxyethyl) ether **D301**
N,N-bis(hydroxyethyl)lauramide **L7**
N,N-bis(β -hydroxyethyl)lauramide **L7**
 bis(2-hydroxyethyl)methylamine **M206**
 bis[hydroxyethylpoly(ethyleneoxy)ethyl]polypropyleneglycol **P218**
 bis(β -hydroxyethyl) sulfide **T129**
 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-21*H*,23*H*-porphine-2,18-dipropanoic acid **H13**
 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-2,18-porphinedipropionic acid **H13**
 bis(2-hydroxy-4-methoxyphenyl)methanone **D349**
 bis(hydroxymethyl)acetylene **B282**
 1,3-bis(hydroxymethyl)-5,5-dimethylhydantoin **D446**
 1,3-bis(hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione **D446**
 bis(hydroxymethyl)furatrizine **D350**
 2,2-bis(hydroxymethyl)-1,3-propanediol **P35**
 2,5-bis(hydroxymethyl)tetrahydrofuran **T73**
 3,3-bis(4-hydroxyphenyl)-1(3*H*)-isobenzofuranone **P81**
 bis(2-hydroxypropyl)amine **D356**
 bis(1-hydroxy-2(1*H*)-pyridinethionato)zinc **Z15**
 bis(8-hydroxyquinolinium) sulfate **H120**
 bis(2-hydroxy-3,5,6-trichlorophenyl)methane **H41**
 bis(4-isocyanatocyclohexyl)methane **M211**
 bis(4-isocyanatophenyl)methane **M214**
 bis(isodecyl) phthalate **D355**
 bis(isooctyloxycarboxylmethylthio) dioctyl stannate **D522**
 2,4-bis(isopropylamino)-6-ethylthio-s-triazine **D551**
 2,4-bis(isopropylamino)-6-methoxy-s-triazine **P288**
 2,4-bis(isopropylamino)-6-(methylthio)-s-triazine **P289**
 bis(isopropyl) ether **D359**
 bis(lauroyloxy)dioctylstannane **D524**
 bis(lauroyloxy)dioctyltin **D524**
 bis(mercaptobenzothiazolato)zinc **Z10**
 1,2-bis(methacryloyloxy)ethane **E119**
 2,2-bis[(methacryloyloxy)methyl]butyl methacrylate **T312**
 1,4-bis(methanesulfonyloxy)butane **B195**
 2,5-bismethoxyethoxy-3,6-bisethyleneimino-1,4-benzoquinone **A267**
 3,6-bis(β -methoxyethoxy)-2,5-bis(ethyleneimino)-*p*-benzoquinone **A267**
 1,2-bis(2-methoxyethoxy)ethane **T296**
 bis(2-methoxyethyl) ether **D338**
 bis(2-methoxyethyl) phthalate **B130**
 2,2-bis(*p*-methoxyphenyl)-1,1,1-trichloroethane **M132**
 1,1-bis(*p*-methoxyphenyl)-2,2,2-trichloroethane **M132**
 bis(methoxythiocarbonyl)disulfide **D463**
 bis(1-methylethyl) adipate **D357**
S-[2-[bis(1-methylethyl)amino]ethyl] *O*-ethyl methylphosphonothioate **V41**
 bis(1-methylethyl)carbamoithioic acid, *S*-(2,3-dichloro-2-propenyl) ester **D69**
 2,3:4,6-bis-*O*-(1-methylethylidene)- α -*L*-xylo-2-hexulofuranosonic acid, sodium salt **D362**
 bis(1-methylethyl) 5-nitro-1,3-benzenedicarboxylate **N178**
 2,6-bis(1-methylethyl)phenol **P314**
O,O-bis(1-methylethyl)*S*-[2-[(phenylsulfonyl)amino]ethyl]phosphorodithioate **B36**
 bis(1-methyl-1-phenylethyl) peroxide **D264**
 bis(2-methylpropyl)amine **D142**
N,N'-bis(1-methylpropyl)-1,4-benzenediamine **D158**
 bis(methylxanthogen)disulfide **D463**
 bismuth gallate, basic **B131**
 bismuth oxygallate **B131**
 bismuth sesquiteroxide **B132**
 bismuth subgallate **B131**
 bismuth telluride **B132**
 bismuth tritelluride **B132**
sym-bis(5-nitro-2-furfurylidene)acetone guanylhydrazone **N184**
 1,5-bis(5-nitro-2-furyl)-3-pentadienone amidinohydrazone **N184**
 1,5-bis(5-nitro-2-furyl)-3-pentadienone guanylhydrazone **N184**
 bisodium carbonate **S52**
 Bisoflex 91 **D508**
 Bisoflex DOA **D514**
 Bisomer CF **H117**

Bisomer DEO **D312**
 Bisomer HPA **H116**
 Bisomer HPMA **H117**
 bis(oxododecyl) peroxide **L9**
 bis(1-oxopropyl)peroxide **D552**
 Bisoxyphen **T122**
 bis(pentabromophenyl) ether **P24**
 bis(pentachlorocyclopentadienyl) **D277**
 bis(1-pentyl) ether **P48**
 bisphenol A **B133**
 bisphenol A diglycidyl ether **B134**
 bis(phenoxarsin-10-yl) ether **O55**
 10,10'-bis(phenoxarsinyl)oxide **O55**
 bisphenyl A diglycidyl ether **B134**
N,N-bis(phosphonomethyl)glycine **G41**
 bis(2-propanol)amine **D356**
trans-1,2-bis(propylsulfonyl)ethylene **B135**
trans-1,2-bis(*n*-propylsulfonyl)ethylene **B135**
 bis(2-pyridylthio)zinc 1,1'-dioxide **Z15**
 bis(quinolin-8-olato)copper **O50**
 bis(8-quinolinolato-*N'*,*O*₈)copper **O50**
 Bisteril **P63**
 bis(2,3,3,3-tetrachloropropyl) ether **B136**
 bis-*N,N,N',N'*-tetramethylphosphorodiamidic anhydride **S9**
 bithiocarbamylhydrazine **D573**
 bithiosemi **M215**
 bis(thiourea) **D573**
 Biston **C61**
 bis(tributylstannane)fumarate **T216**
 bis(tributylstannyl) oxide **T219**
 bis(tributyltin)fumarate **T216**
 bis(tributyltin) oxide **T219**
 bis(tributyltin) phthalate **T220**
 bis(tributyltin) succinate **T221**
 bis(tri-*n*-butyltin) succinate **T221**
 bis(tributyltin) sulfide **T222**
 bis(trifluoroacetic) anhydride **T291**
 bis(trifluoromethyl)methanol **H47**
 bis(trimethylsilyl)amine **H52**
 bis(2,4,6-trinitrophenyl)amine **D550**
 bis(tripropyltin) oxide **T344**
 bis[tris(2-methyl-2-phenylpropyl)tin] oxide **F7**
 bisulfane **B195**
 bitertanol **B137**
 bithionolate sodium **S49**
 Bitionol **T122**
 bitoscanate **B138**
 bitter almond oil camphor **B64**
 bitumen **A249**
 biviny **B197**
 B-I-K **U12**
 black lead **G45**
 black leaf **N55**
 Bladafum **S147**
 Bladan **T68**
 Blade **O47**

Bladex **C480**
 Blanc Fixe **B24**
 Bla-S **B139**
 blasticidin-S **B139**
 blasting gelatin **G26**
 Blattanax **P315**
 Blattlausfrei **B223**
 Blattlaus Spray **D376**
 Blazer **A30**
 bleomycin **B140**
 Blitex **F8**
 Bloc **F4**
 blood sugar **G17**
 Blotic **P304**
 blue asbestos **C465**
 blue 15B **P176**
 Blue Base Irga B **D95**
 Blue Base NB **D95**
 Blue BN Base **D95**
 blue copper **C441**
 Blue Oil **A209**
 Blue-ox **Z14**
 blue powder **Z2**
 Blue VRS **C386**
 Bo-Ana **F1**
 boldine dimethyl ether **G15**
 boletic acid **F115**
 Boliron **L50**
 Bolls-Eye **C1**
 Bolstar **S159**
 Bonaform **T50**
 Bonalan **B29**
 Bonare **O48**
 Booster **C131**
 Boot Hill **B152**
 Boramae **F6**
 borane (B₂H₆) **D121**
 borate(1-), tetrafluoro-, lead(II) **L21**
 borate(1-), tetrahydro-, sodium **S50**
 borax **B141**
 borax **S96**
 borax decahydrate **B141**
 borax glass **S96**
 Bordeaux mixture **B142**
 Borderclear **L34**
 Bordermaster **M32**
 Bordocure **B142**
 Bordolex **B142**
 borester **T308**
 Borial **I62**
 boric acid, disodium salt **S96**
 boric acid, trimethyl ester **T308**
 boric anhydride **B144**
endo-2-bornanol **B143**
 2-bornanone **C50**
 borneol **B143**
 bornyl alcohol **B143**

Borocil **B151**
 boroethane **D121**
 borol **S50**
 boron bromide **B145**
 boron chloride **B146**
 boron ethoxide **E101**
 boron fluoride **B147**
 boron hydride **D37**
 boron hydride (B₂H₆) **D121**
 boron oxide **B144**
 boron sesquioxide **B144**
 boron sodium oxide **S96**
 boron tribromide **B145**
 boron trichloride **B146**
 boron triethoxide **E101**
 boron trifluoride **B147**
 boron trifluoride diethyl ether **B148**
 boron trifluoride diethyl etherate **B148**
 boron trifluoride dimethyl etherate **B149**
 boron trifluoride etherate **B148**
 Bosban **X4**
 Boxer **E72**
 BPMC **F12**
 Brake **F86**
 Brasoran **A265**
 Brassicol **Q12**
 Bravo **C286**
 Bray's Emulsion **C456**
 Brazil wax **C87**
 Brebent **B39**
 Bregel **B39**
 Brek **C131**
 Brenox **D560**
 Brestan **F26**
 Brestan 60 **F25**
 brestanol **T340**
 brick oil **C453**
 Brigade **B109**
 Brilliant Blue **C411**
 Brilliant Fast Oil Yellow **M320**
 Brilliant Green B **C400**
 Brilliant Ponceau 3R **C394**
 brilliant yellow **D96**
 brimstone **S149**
 British Anti-Lewisite **D369**
 BRL-2333 **A192**
 Brocasipil **O35**
 Brocum **B150**
 Brodal **D327**
 Brodan **C313**
 brodifacoum **B150**
 Broenners acid **A134**
 bromacil **B151**
 bromadiolone **B152**
 bromallylene **A76**
 Bromax **B151**
 Bromazil **I4**
 Brombloom **H91**
 bromchlophos **N3**
 Bromcholitin **G15**
 bromethalin **B153**
 Bromex **N3**
 bromic acid, barium salt **B7**
 bromic acid, potassium salt **P241**
 bromic acid, sodium salt **S51**
 bromic ether **B175**
 bromine **B154**
 bromine chloride **B155**
 bromine cyanide **C483**
 bromine monochloride **B155**
 bromine pentafluoride **B156**
 bromine trifluoride **B157**
 Brominil **B189**
 bromoacetic acid **B158**
 bromoacetic acid, methyl ester **M171**
 bromoacetonitrile **B159**
 4-bromoaniline **B160**
p-bromoaniline **B160**
 4-bromobenzenamine **B160**
 bromobenzene **B161**
 α-bromobenzyl cyanide **B162**
 α-bromobenzyl nitrile **B162**
 3-(3-(4'-bromo-(1,1'-biphenyl)-4-yl)3-hydroxy-1-phenylpropyl)-4-hydroxy-2*H*-1-benzopyran-2-one **B152**
 3-[3-(4'-bromo[1,1'-biphenyl]-4-yl)-1,2,3,4-tetrahydro-1-naphthalenyl]-4-hydroxy-2*H*-1-benzopyran-2-one **B150**
 3-(3-(4'-bromobiphenyl-4-yl)-1,2,3,4-tetrahydronaphth-1-yl)-4-hydroxycoumarin **B150**
 2-bromo-2-(bromomethyl)pentanedinitrile **B163**
 4-bromo-α-(4-bromophenyl)-α-hydroxybenzeneacetic acid 1-methylethyl ester **B187**
 1-bromobutane **B164**
 2-bromobutane **B165**
 bromobutide **B166**
 5-bromo-3-*sec*-butyl-6-methyluracil **B151**
 bromochloride **B155**
 bromochloroacetonitrile **B167**
 bromochlorodifluoromethane **B168**
 3-bromo-1-chloro-5,5-dimethylhydantoin **B169**
 3-bromo-1-chloro-5,5-dimethyl-2,4-imidazolidinedione **B169**
 1-bromo-2-chloroethane **B170**
 bromochloromethane **B171**
O-(4-bromo-2-chlorophenyl) *O*-ethyl *S*-propyl phosphorothioate **P279**
 3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea **C116**
N'-(4-bromo-3-chlorophenyl)-*N*-methoxy-*N*-methylurea **C116**
 1-bromo-3-chloropropane **B172**
 bromochlorotrifluoroethane **H4**
 2-bromo-2-chloro-1,1,1-trifluoroethane **H4**

bromocyan **C483**
 bromocyanogen **C483**
 Bromodialone **B152**
 bromodichloromethane **B173**
O-(4-bromo-2,5-dichlororophenyl) *O,O*-methyl phenyl-phosphonothioate **L35**
 2-bromo-*N*-(α,α -dimethylbenzyl)-3,3-dimethylbutyramide **B166**
 4-bromodiphenyl ether **B174**
 1-bromo-2,3-epoxypropane **E32**
 bromoethane **B175**
 bromoethanoic acid **B158**
 α -bromoethanoic acid **B158**
 bromoethene **V28**
 2-bromo-2-ethylbutyrylurea **C85**
 bromoethylene **V28**
 bromofenoxim **B176**
 Bromoflor **E63**
 bromoform **B177**
 bromohydrin **E32**
 Bromol **T207**
 bromomethane **B178**
 3-bromo-3-(4-methoxybenzoyl)acrylic acid, sodium salt **C547**
 (bromomethyl)benzene **B92**
 1-bromo-3-methylbutane **B179**
 bromomethyl cyanide **B159**
 (bromomethyl)ethylene oxide **E32**
 5-bromo-6-methyl-3-(1-methylpropyl)-2,4(1*H*,3*H*)-pyrimidinedione **B151**
 2-(bromomethyl)oxirane **E32**
 2-bromonitrobenzene **B180**
 4-bromonitrobenzene **B181**
 2-bromo-2-nitroethenylbenzene **B182**
 2-bromo-2-nitro-1,3-propanediol **B190**
 β -bromo- β -nitrostyrene **B182**
 β -bromo- β -nitrotrimethylene glycol **B190**
 bromophenoxim **B176**
 1-bromo-4-phenoxybenzene **B174**
 α -bromophenylacetone nitrile **B162**
p-bromophenylamine **B160**
p-bromophenyl bromide **D124**
 3-(α -(*p*-bromophenyl)- β -hydroxyphenethyl)benzyl)-4-hydroxycoumarin **B152**
 bromophenylmethane **B92**
 3-(4-bromophenyl)-1-methoxy-1-methylurea **M322**
N'-(4-bromophenyl)-*N*-methoxy-*N*-methylurea **M322**
 4-bromophenyl phenyl ether **B174**
 bromophos **B183**
 bromophos-ethyl **B184**
 bromophos-methyl **B183**
 bromopicrin **T206**
 1-bromopropane **B185**
 2-bromopropane **B186**
 1-bromo-2-propene **A76**
 3-bromo-1-propene **A76**
 bromopropylate **B187**
 3-bromopropyl chloride **B172**
 3-bromopropylene **A76**
 Bromorat **B152**
 α -bromotoluene **B92**
 ω -bromotoluene **B92**
 α -bromo- α -tolunitrile **B162**
 bromotrifluoromethane **B188**
 bromoxynil **B189**
 Bromurex **M322**
 bronopol **B190**
 Bronosal **B190**
 Bronotak **B190**
 bronze powder **C429**
 bronze scarlet CA **D27**
 brown copper oxide **C440**
 BRP **N3**
 brucine **B191**
 (–)-brucine **B191**
 Brufen **I2**
 Brush-off **M328**
 BZT **B51**
 BTO **T219**
 bualta **P217**
 Bubond 60 **P217**
 Buctril **B189**
 Bud Nip **C312**
 bufopzinc zinc sulfate **Z17**
 Buhach **P354**
 Bulkaloid **M185**
 Bullit **P209**
 buminafos **B192**
 Bumper **P306**
 bupirimate **B193**
 buprofezin **B194**
 Buracyl **L34**
 Buranit **C498**
 burex **C131**
 burnt alum **A105**
 burnt lime **C37**
 Burstane **L59**
 Burtolin **M14**
 Busan 1060 **H51**
 Busan 77 **P217**
 Busan 85 **P247**
 Buster **G18**
 Bustren **P231**
 busulfan **B195**
 butachlor **B196**
 Butacide **P204**
 buta-1,3-diene **B197**
 1,3-butadiene **B197**
 butadiene diepoxide **D278**
 1,3-butadiene diepoxide **D278**
 butadiene dimer **V31**
 butadiene dioxide **D278**
 butadiene sulfone **S144**
 2,3-butadione **B209**

Butafume **B240**
 Butalidon **P96**
 Butamide **T171**
 butamifos **B198**
 butanal **B283**
 butanal oxime **B284**
 butanamide, *N*-(aminocarbonyl)-2-bromo-2-ethyl- **C85**
 butanamide, 2-bromo-3,3-dimethyl-*N*-(1-methyl-1-phenylethyl)- **B166**
 butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[*N*-(2,4-dimethylphenyl)-3-oxo- **C419**
 1-butanamine **B239**
 2-butanamine **B240**
 1-butanamine, *N*-methyl- **M180**
 butane **B199**
iso-butane **I84**
n-Butane **B199**
 butane, 1-bromo- **B164**
 1-butanecarboxylic acid **V2**
 butane, 1-chloro **B251**
 1,3-butanediamine **B200**
 1,4-butanediamine **B201**
 1,4-butanediamine, *N*-(3-aminopropyl)- **S106**
 1,4-butanedicarboxylic acid **A48**
 butane diepoxide **D278**
 butanedinitrile **S130**
 butanedioic acid **S128**
 butanedioic acid, compound with *N,N*-dimethyl-2-[1-phenyl-1-(2-pyridinyl)ethoxy]ethanamine (1:1) **D599**
 butanedioic acid, 2,3-dihydroxy-, diammonium salt **A188**
 butanedioic acid, [(dimethoxyphosphinyl)thio]-, diethyl ester **M10**
 butanedioic acid, mono(2,2-dimethylhydrazide) **D21**
 butanedioic anhydride **S129**
 1,2-butanediol **B202**
 1,3-butanediol **B203**
 1,4-butanediol **B204**
 2,3-butanediol **B205**
 1,3-butanediol diacrylate **B206**
 1,4-butanediol diacrylate **B207**
 1,4-butanediol diglycidyl ether **B208**
 1,4-butanediol dimethanesulfonate **B195**
 2,3-butanedione **B209**
 2,2'-[1,4-butanediylbis(oxymethylene)bisoxyrane] **B208**
 butane, 1-isocyanato **B264**
 butanenitrile **B289**
n-butanenitrile **B289**
 butanenitrile, 4-chloro- **C180**
 1,2-butane oxide **E36**
 1,4-butane sultone **B210**
 1,2,3,4-butanetetrol, 1,4-dimethanesulfonate, [*S*-(*R,R*)]- **T195**
 1-butanethiol **B211**
n-butanethiol **B211**
 Butanex **B196**
 butanoic acid **B285**
 butanoic acid anhydride **B286**
 butanoic acid, 3-methyl-, butyl ester **B265**
 butanoic acid, 1-methylethyl ester **I123**
 butanoic acid, pentyl ester **A197**
 butanoic acid, 2,2,2-trichloro-1-dimethoxyphosphinyl)ethyl ether **B224**
 butanoic anhydride **B286**
 1-butanol **B212**
 2-butanol **B213**
tert-butanol **B214**
 2-butanol, 4-(dimethylethylamino)-3-methyl-1,2-diphenyl-, propionate (ester), (-)- **L39**
 1,4-butanolide **B288**
 butan-2-one **M220**
 2-butanone **M220**
 2-butanone, 3-(methylsulfonyl)-*O*-[(methylamino)carbonyl]oxime **B225**
 2-butanone, 3-(methylthio)-*O*-[(methylamino)carbonyl]oxime **B223**
 2-butanone oxime **M221**
 2-butanone peroxide **M222**
 Butanox **B196**
 butanoyl chloride **B290**
 Butapirone **O63**
trans-2-butenal **C467**
 butene-2 **B216**
 1-butene **B215**
cis-2-butene **B216**
trans-2-butene **B217**
cis-butenedioic acid **M12**
 (*E*)-2-butenedioic acid **F115**
trans-2-butenedioic acid **F115**
 (*Z*)-butenedioic acid **M12**
 2-butenedioic acid, (*Z*)-, dimethyl ester **D426**
 2-butenedioic acid (*E*)-, iron (2+) salt (1:1) **I72**
cis-butenedioic anhydride **M13**
 1-butene oxide **E36**
 α -butenoic acid **C468**
 (*Z*)-2-butenic acid **C468**
 2-butenic acid, 3-[(dimethoxyphosphinyl)oxy]-, 1-phenylethyl ester, (*E*)- **M167**
 2-butenic acid, 3-[(ethylamino)methoxyphosphinothioyl]oxy]-, 1-methylethyl ester **P304**
 2-butenic acid, 3-methyl-2-(1-methylpropyl)-4,6-dinitrophenyl ester **B111**
 but-2-en-1-ol **C470**
 but-3-en-1-ol **B219**
 but-3-en-2-ol **B220**
 2-buten-1-ol **C470**
 3-buten-1-ol **B219**
 3-buten-2-ol **B220**
 Δ^2 -1-butenol **C470**
 Δ^3 -1-butenol **B219**
 Δ^3 -2-butenol **B220**
E-but-2-en-1-ol **B218**
trans-but-2-en-1-ol **B218**
trans-2-buten-1-ol **B218**

3-buten- β -lactone **D363**
 1-buten-3-one **M318**
 3-buten-2-one **M318**
 3-buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (E)-**I57**
 2-butenyl chloride **C176**
 3-butenyl chloride **C179**
 buthiobate **B221**
 Butifos **T209**
 2-butine **C469**
 butinox **T219**
 Butiphos **M89**
 Butisan S **M98**
 Butizyl **M34**
 butobarbitone **B222**
 butocarboxim **B223**
 butonate **B224**
 butox **D46**
 Butoxone **M34**
 1-butoxybutane **D145**
 butoxycarbonyl chloride **B254**
 butoxycarboxim **B225**
 butoxydiglycol **B227**
 1-butoxy-2,3-epoxypropane **B259**
 2-butoxyethanol **B226**
 2-butoxy-1-ethanol **B226**
 2-butoxyethanol acetate **B229**
 2-butoxyethanol phosphate **T348**
 butoxyethene **B280**
 2-(2-butoxyethoxy)ethanol **B227**
 2-(2-butoxyethoxy)ethanol acetate **B228**
 α -[2-(2-*n*-butoxyethoxy)ethoxy]-4,5-methylenedioxy-2-propyltoluene **P204**
 5{[2-(2-butoxyethoxy)ethoxy)methyl]-6-propyl-1,3-benzodioxole **P204**
 2-butoxyethyl acetate **B229**
 (butoxymethyl)oxirane **B259**
 butoxypropanol **B230**
 1-butoxy-2-propanol **B231**
 butralin **B232**
 Buttercup Yellow **Z7**
 butter of zinc **Z6**
 Butter Yellow **C424**
 Butter Yellow **M320**
 butyglycol **B226**
 butyl acetate **B233**
 2-butyl acetate **B234**
sec-butyl acetate **B234**
tert-butyl acetate **B235**
 butylacetic acid **H64**
 butyl acetoacetate **B236**
 butyl acid phosphate **B237**
 butyl acrylate **B238**
 butyl adipate **D140**
n-butyl alcohol **B212**
sec-butyl alcohol **B213**
tert-butyl alcohol **B214**
sec-butyl alcohol acetate **B234**
 butylaldehyde **B283**
 butylamine **B239**
n-butylamine **B239**
 (*RS*)-*sec*-butylamine **B240**
sec-butylamine **B240**
tert-butylamine **B241**
 butylamine, *N*-methyl- **M180**
N-[(butylamino)carbonyl]-4-methylbenzenesulfonamide **T171**
 2-(*tert*-butylamino)-4-chloro-6-ethylamino-*s*-triazine **T24**
 1-butylaminocyclohexanephosphonic acid, butyl ester **B192**
 2-(*tert*-butylamino)-4-(ethylamino)-6-methylthio-*s*-triazine **T25**
 2-(*tert*-butylamino)-(4-hydroxy-3-hydroxymethylphenyl)-ethanol **S3**
 α 1-[(*tert*-butylamino)methyl-4-hydroxy-*m*-xylene- α,α' -diol **S3**
N-butylaniline **B242**
N-(*n*-butyl)aniline **B242**
 butylate **B243**
 butylated hydroxyanisole **B244**
 butylated hydroxytoluene **B245**
 butylate-2,4,5-T **B279**
N-butylbenzenamine **B242**
 butylbenzene **B246**
n-butylbenzene **B246**
tert-butylbenzene **B247**
N-butylbenzenesulfonamide **B248**
 4-*tert*-butylbenzoic acid **B249**
p-*tert*-butylbenzoic acid **B249**
 butyl benzyl phthalate **B94**
 butyl bromide **B164**
sec-butyl bromide **B165**
N-butyl-1-butanamine **D141**
 butyl butanoate **B250**
 2-butylbutanoic acid **E127**
 butyl, 4-*tert*-butylbenzyl-*N*-(3-pyridyl)dithiocarbonimidate **B221**
N-*sec*-butyl-4-*tert*-butyl-2,6-dinitroaniline **B232**
 butyl butyrate **B250**
n-butylcarbinol **P41**
 butyl carbinol 6-propylpiperonyl ether **P204**
 butylcarbitol **B227**
 butyl carbitol **B227**
 butyl carbitol acetate **B228**
n-butylcarbonyl chloride **A198**
 butyl cellosolve **B226**
 butyl cellusolve acetate **B229**
 butyl chloride **B251**
n-butylchloride **B251**
sec-butyl chloride **B252**
tert-butyl chloride **B253**
 butylchlorocarbonate **B254**
*N*2-*tert*-butyl-6-chloro-*N*4-ethyl-1,3,5-triazine-2,4-diamine **T24**

butyl chloroformate **B254**
n-butyl chloroformate **B254**
 3-*tert*-butyl-5-chloro-6-methyluracil **T20**
 4-*tert*-butyl-2-chlorophenyl-*N*-methyl *O*-
 methylphosphoramidate **C471**
tert-butyl chromate **B255**
tert-butylchromate (VI) **B255**
tert-butylcyclohexane **D415**
 2-*tert*-butyl-4-(2,4-dichloro-5-isopropoxyphenyl) Δ^2 -1,3,4-
 oxadiazolin-5-one **O44**
 butyl dichlorophenoxyacetate **D4**
 1-butyl-3-(3,4-dichlorophenyl)-1-methylurea **N32**
N-butyl-*N'*-(3,4-dichlorophenyl)-*N*-methyl urea **N32**
 (\pm)- α -butyl- α -(2,4-dichlorophenyl)-1*H*-1,2,4-triazole-1-
 ethanol **H43**
 butyl digol **B227**
 butyl 2,3-dihydro-2,2-dimethylbenzofuran-7-yl *N,N'*-
 dimethyl-*N,N'*-thiocarbamate **F125**
 2-*tert*-butyl-1,4-dimethoxybenzene **B256**
 5-butyl-2-(dimethylamino)-6-methyl-4-pyrimidinol **D375**
 5-butyl-2-(dimethylamino)-6-methyl-4(1*H*)-pyrimidinone
D375
 butyl[4-(1,1-dimethylethyl)phenyl]methyl-3-
 pyridinylcarbonimidodithioate **B221**
t-butyl(*E*)- α -(1,3-dimethyl-5-phenoxy-pyrazol-4-
 ylmethyleneamino-oxy)-*p*-toluate **F21**
 1-*tert*-butyl-3,5-dimethyl-2,4,6-trinitrobenzene **M358**
 2-*sec*-butyl-4,6-dinitrophenol **D510**
 2-*tert*-butyl-4,6-dinitrophenol **D512**
o-*tert*-butyl-4,6-dinitrophenol **D512**
 2-*sec*-butyl-4,6-dinitrophenyl acetate **D511**
 2-*sec*-butyl-4,6-dinitrophenyl isopropylcarbonate **D504**
 2-*sec*-butyl-4,6-dinitrophenyl 3-methylcrotonate **B111**
 4-butyl-1,2-diphenyl-3,5-pyrazolidinedione **P96**
 butylene **B215**
 butylene-1 **B215**
 butylene-2 **B216**
 α -butylene **B215**
 β -butylene **B216**
 β -butylene **B217**
 γ -butylene **I86**
 butylene diacrylate **B207**
 1,3-butylene diacrylate **B206**
 2-butylene dichloride **D200**
 2-butylene dichloride **D201**
 1,2-butylene glycol **B202**
 1,3-butylene glycol **B203**
 1,4-butylene glycol **B204**
 2,3-butylene glycol **B205**
 β -butylene glycol **B203**
 1,3-butylene glycol diacrylate **B206**
 1,4-butylene glycol diacrylate **B207**
 butylene hydrate **B213**
 1-butylene oxide **E36**
 α -butylene oxide **E36**
 1,4-butylene sulfone **B210**
 butyl 2,3-epoxypropyl ether **B259**
 butyl ethanoate **B233**
n-butyl ether **D145**
 butylethylacetaldehyde **E125**
 butylethylacetic acid **E127**
 5-butyl-2-ethylamino-6-methylpyrimidin-4-yl dimethyl
 sulfamate **B193**
 5-butyl-5-ethylbarbituric acid **B222**
N-*tert*-butyl-*N'*-(4-ethylbenzoyl)-3,5-
 dimethylbenzohydrazide **T12**
 butylethylcarbamothioic acid, *S*-propyl ester **P17**
N-butyl-*N*-ethyl-2,6-dinitro-4-trifluoromethylaniline **B29**
N-butyl-*N*-ethyl-2,6-dinitro-4-
 (trifluoromethyl)benzenamine **B29**
 butyl ethylene **H70**
 butyl ethyl ether **B257**
 butyl ethyl ketone **H24**
n-butyl ethyl ketone **H24**
*N*²-*tert*-butyl-*N*⁴-ethyl-6-methoxy-1,3,5-triazine-2,4-diamine
T23
*N*²-*tert*-butyl-*N*⁴-ethyl-6-methylthio-1,3,5-triazine-2,4-
 diamine **T25**
 5-butyl-5-ethyl-2,4,6(1*H*,3*H*,5*H*)pyrimidinetrione **B222**
 butylethylthiocarbamic acid, *S*-propyl ester **P17**
N-butyl-*N*-ethyl- α,α,α -trifluoro-2,6-dinitro-*p*-toluidine **B29**
 butyl formate **B258**
n-butyl formate **B258**
 butyl glycidyl ether **B259**
tert-butyl glycidyl ether **B260**
 butylglycol **B226**
 butylglycol acetate **B229**
 butyl hydrogen phthalate **M341**
tert-butyl hydroperoxide **B261**
tert-butylhydroquinone **B262**
 butylhydroxide **B212**
tert-butyl hydroxide **B214**
 butyl 4-hydroxybenzoate **B269**
 butyl *p*-hydroxybenzoate **C351**
 butyl *p*-hydroxybenzoate **B269**
 4-butyl-1-(4-hydroxyphenyl)-2-phenyl-3,5-
 pyrazolidinedione **O63**
 butyl α -hydroxypropionate **B266**
sec-butylidenebis[*tert*-butyl peroxide] **D151**
 1-butylimidazole **B263**
N-butylimidazole **B263**
 2-*tert*-butylimino-3-isopropyl-5-phenyl-3,4,5,6-tetrahydro-
 2*H*-1,3,5-thiadiazin-4-one **B194**
 butyl iodide **I46**
 2-butyl iodide **I47**
n-butyliodide **I46**
sec-butyl iodide **I47**
tert-butyl iodide **I54**
 butyl isocyanate **B264**
n-butyl isopentanoate **B265**
 butyl isovalerate **B265**
 butyl lactate **B266**
n-butyl lactate **B266**
 butyl mercaptan **B211**

butyl methacrylate **B267**
 butylmethylamine **M180**
 butyl 3-methylbutyrate **B265**
 butylmethylcarbinol **H66**
 6-*tert*-butyl-3-methyl-2,4-dinitroanisole **M357**
tert-butyl methyl ether **M181**
 butyl methyl ketone **H67**
tert-butyl methyl ketone **P192**
 butyl 2-methyl-2-propenoate **B267**
 butyl nitrate **B268**
N-butyl-*N*-nitroso-1-butanamine **N146**
 butyl oxide **D145**
 butyl oxirane **E38**
 2-butyloxirane **E38**
 3-[4-(2-*tert*-butyl-5-oxo- Δ^2 -1,3,4-oxadiazolin-4-yl)-3-chlorophenyl]-1,1-dimethylurea **D368**
 butylparaben **B269**
 Butyl Parasept NF **B269**
tert-butyl peracetate **B270**
tert-butyl perbenzoate **B271**
tert-butyl perisobutyrate **B272**
tert-butyl perisononanoate **B274**
tert-butyl peroxide **D150**
tert-butyl peroxyacetate **B270**
tert-butyl peroxybenzoate **B271**
sec-butyl peroxydicarbamate **D153**
 butyl peroxydicarbonate **D152**
tert-butyl peroxyisobutyrate **B272**
tert-butyl peroxyipivalate **B273**
tert-butyl peroxy-3,5,5-trimethylhexanoate **B274**
tert-butylperpivalate **B273**
 butylphen **B276**
 4-*tert*-butylphenethyl quinazolin-4-yl ether **F6**
 2-*sec*-butylphenol **B275**
 4-*tert*-butylphenol **B276**
 2-*sec*-butylphenyl methylcarbamate **F12**
cis-4-[3-(4-*tert*-butylphenyl)-2-methylpropyl]-2,6-dimethylmorpholine **F20**
 (\pm)-1-[3-(*p*-*tert*-butylphenyl)-2-methylpropyl] piperidine **F19**
 butyl phosphoric acid **B237**
 butyl phosphorothioate **T209**
n-butyl phthalate **D160**
 butylpropanoate **B277**
 butyl 2-propenoate **B238**
 butyl propionate **B277**
n-butylpropionate **B277**
 1-(5-*tert*-butyl-1,3,4-thiadiazol-2-yl)-1,3-dimethylurea **T13**
n-butyl thioalcohol **B211**
S-*tert*-butylthiomethyl *O,O*-diethyl phosphorodithioate **T22**
 4-*tert*-butyltoluene **B278**
p-*tert*-butyltoluene **B278**
 1-butyl-3-(*p*-tolylsulfonyl)urea **T171**
 butyl 2,4,5-trichlorophenoxyacetate **B279**
 (\pm)-butyl 2-[4-[5-(trifluoromethyl)-2-pyridinyloxy]phenoxy]propanoate **F38**

butyl (*R*)-2-[4-[5-(trifluoromethyl)-2-pyridinyloxy]phenoxy]propanoate **F39**
 butyl-(*RS*)-2-[4-(5-trifluoromethyl-2-pyridyloxy) phenoxy]propanoate **F38**
tert-butyltrimethylperoxyacetate **B273**
tert-butyl 3,5,5-trimethylperoxyhexanoate **B274**
 5-*tert*-butyl-2,4,6-trinitro-*m*-xylene **M358**
 butyl vinyl ether **B280**
 6-*tert*-butyl-2,4-xyleneol **D405**
 1-butyne **B281**
 2-butyne **C469**
 1,4-butyne diol **B282**
 2-butyne diol **B282**
 2-butyne-1,4-diol **B282**
 butynorate **D163**
 1-butyne-3-yl *m*-chlorophenylcarbamate **C117**
 butyraldehyde **B283**
 butyraldehyde oxime **B284**
n-butyraldehyde oxime **B284**
 butyraldoxime **B284**
N-butyraldoxime **B284**
 butyric acid **B285**
 butyric acid anhydride **B286**
n-butyric acid anhydride **B286**
 butyric acid chloride **B290**
 butyric acid, isopropylester **I123**
 butyric acid lactone **B288**
 butyric acid nitrile **B289**
 butyric acid, pentyl ester **A197**
 butyric alcohol **B212**
 butyric aldehyde **B283**
 butyric anhydride **B286**
 butyric ether **E105**
 butyrin **T223**
 butyrylase **L51**
 β -butyrolactone **B287**
 γ -butyrolactone **B288**
 butyronitrile **B289**
 butyryl chloride **B290**
n-butyryl chloride **B290**
 butyryl oxide **B286**
 butyryl triglyceride **T223**
 Buvidol **F97**
 Buvilan **E56**
 Bygran **T14**
 C.1. 77402 **C440**
 C 400 **P3**
 C46 **H34**
 C516 **T316**
 C601 **H40**
 CA69-15 **I59**
 Cabral **P140**
 cacodylic acid **C1**
 cacodylic acid sodium salt **S63**
 Cactinomycin **A45**
 caddy **C5**
 cadmium **C2**

cadmium acetate **C3**
 cadmium bromide **C4**
 cadmium chloride **C5**
 cadmium chloride monohydrate **C6**
 cadmium diacetate **C3**
 cadmium dibromide **C4**
 cadmium dichloride **C5**
 cadmium diiodide **C10**
 cadmium fluoride **C7**
 cadmium fluorosilicate **C8**
 cadmium fluorure (French) **C7**
 cadmium formate **C9**
 cadmium fume **C11**
 cadmium hexafluorosilicate **C8**
 cadmium iodide **C10**
 cadmium monoxide **C11**
 Cadmium Orange **C14**
 cadmium oxide **C11**
 cadmium oxide fume **C11**
 cadmium stearate **C12**
 cadmium sulfate **C13**
 cadmium sulfide **C14**
 Cadol **D570**
 cadusafos **C15**
 caesium **C16**
 caesium hydroxide **C17**
 caesium nitrate **C18**
 caesium nitrate (1:1) **C18**
 caffeic acid **C19**
 caffeine **C20**
 Cafudan **C59**
 Caid **C238**
 cairox **P260**
 Cajeputol **C343**
 Calamine **Z5**
 calcia **C37**
 Calcicat **C21**
 calcic liver of sulfur **C46**
 Calcid **C30**
 calcined baryta **B14**
 calcined diatomite **C464**
 calciol **C323**
 calcium **C21**
 calcium acetylde **C24**
 calcium arsenate **C22**
 calcium arsenite **C23**
 calcium carbide **C24**
 calcium carbimide **C29**
 calcium carbonate **C25**
 calcium chlorate **C26**
 calcium chloride 5-chloro-2-methyl-3(2*H*)-isothiazolone
 (1:1) complex **C213**
 calcium chlorite **C27**
 calcium chlorohydrochlorite **C34**
 calcium chromate **C28**
 calcium chromate(vi) **C28**
 calcium chrome yellow **C28**

calcium chromium oxide **C28**
 calcium cyanamide **C29**
 calcium cyanide **C30**
 calcium dicarbide **C24**
 calcium difluoride **F80**
 calcium dinitrate **C36**
 calcium dioxide **C39**
 calcium disodium detate **E4**
 calcium disodium EDTA **E4**
 Calcium Disodium Versenate **E4**
 calcium dithionite **C31**
 calcium dodecylbenzenesulfonate **C32**
 calcium EDTA **E4**
 calcium hydrate **C33**
 calcium hydrosilicate **C43**
 calcium hydrosulfite **C31**
 calcium hydroxide **C33**
 calcium hypochlorite **C34**
 calcium *o*-iodoxybenzoate **C35**
 calcium monochromate **C28**
 calcium monosilicate **C43**
 calcium monosulfide **C46**
 calcium nitrate **C36**
 calcium orthoarsenate **C22**
 calcium oxide **C37**
 calcium permanganate **C38**
 calcium peroxide **C39**
 calcium phosphate **C40**
 calcium phosphate tribasic **C40**
 calcium phosphide **C41**
 calcium polysilicate **C43**
 calcium polysulfides **C42**
 calcium silicate **C43**
 calcium sulfate **C44**
 calcium sulfate dihydrate **C45**
 calcium sulfide **C42**
 calcium sulfide **C46**
 Calcocid Green S **C389**
 Calcocid Scarlet 2R **C395**
 Calcozine Fuchsine HO **M1**
 Calcozine Magenta N **C402**
 Calcyan **C30**
 C-8 aldehyde **O8**
 Caldine **N208**
 Caldon **D510**
 Calgon **S69**
 Calibre **H80**
 Calin **L50**
 calirus **B31**
 Calliact **T226**
 Callidim **D376**
 Calligal **M40**
 Callimal **M11**
 calochlor **M71**
 calomel **C47**
 Caloxol **C37**
 calx **C37**

Camal **C298**
 camcopat **P243**
endo-2-camphanol **B143**
 2-camphanone **C50**
 camphechlor **C48**
 camphene **C49**
 camphol **B143**
 camphor **C50**
 (1*R*)-(+)-camphor **C51**
 (1*S*)-(-)-camphor **C52**
D-camphor **C51**
DL-camphor **C53**
L-(-)-camphor **C52**
 (-)-camphor **C52**
 (+)-camphor **C51**
 (±)-camphor **C53**
 Campogran **F130**
 Camposan **E63**
 Campoviton 6 **P359**
 Canary Yellow **Q10**
 Cancror **O50**
 Candex **N210**
 Candor **C68**
 canescine **D58**
 cane sugar **S131**
 Canfelzo **Z12**
 Canguard 409 **B190**
 Canguard 454 **H51**
 Canogard **D258**
 cantharides camphor **C54**
 cantharidin **C54**
 cantharidine **C54**
 cantharone **C54**
 Canthaxanthin **C413**
 Cap **C59**
 Cap **C139**
 Capfos **F99**
 capmul **P227**
 capraldehyde **D40**
 caproaldehyde **H59**
n-caproic acid **H64**
 caproic aldehyde **H59**
 caprolactam **C55**
ε-caprolactam **C55**
 capronic acid **H64**
 caproyl alcohol **H65**
 capryl alcohol **O14**
 capryl aldehyde **O8**
 capryldinitrophenyl crotonate **D505**
 caprylic acid **O12**
 caprylic acid triglyceride **T224**
 caprylic alcohol **O13**
sec-caprylic alcohol **O14**
 caprylic aldehyde **O8**
 capsanthin **C56**
 capsorubin **C57**
 captafol **C58**
 captan **C59**
 captax **M61**
 Capture **B109**
 Capture **C542**
 Caraz **I59**
 carbachol chloride **C60**
 Carbacholin **C60**
 Carbal **C63**
 carbamaldehyde **F101**
 carbamazepine **C61**
 carbamic acid, [(4-aminophenyl)sulfonyl]-, methyl ester **A251**
 carbamic acid, 1*H*-benzimidazol-2-yl-, methyl ester **C65**
 carbamic acid, [(dibutylamino)thio]methyl-, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl ester **C83**
 carbamic acid, diisobutylthio-, *S*-ethyl ester **B243**
 carbamic acid, dimethyldithioanhydrosulfide **M348**
 carbamic acid, (1,1-dimethylethyl)-, 3-[[[(dimethylamino)carbonyl]amino]phenyl ester **K4**
 carbamic acid, methyl-, *m*-cym-5-yl ester **P286**
 carbamic acid, methyl-, 2,3-(isopropylidenedioxy)phenyl ester **B28**
 carbamic acid, (3-methylphenyl)-, 3-[(methoxycarbonyl)-amino]phenyl ester **P78**
 carbamic acid, 2-methyl-2-propyltrimethylene ester **M57**
 carbamic acid, propyl ester **P325**
 carbamic acid, zinc salt (1:1) **Z5**
 carbamic chloride, diethyl- **D296**
 carbamide **U12**
 carbamimidosenoic acid **S21**
 Carbamite **D297**
 carbamodithioic acid, diethyl-, sodium salt **D575**
 carbamonitrile **C479**
 carbamothioic acid, bis(2-methylpropyl)-, *S*-ethyl ester **B243**
 carbamothioic acid, bis(1-methylpropyl)-*S*-(phenylmethyl) ester **T162**
 carbamothioic acid, cyclohexylethyl-, *S*-ethyl ester **C498**
 carbamothioic acid, *S,S'*-[2-(dimethylamino)-1,3-propanediyl] ester, monohydrochloride **C92**
o-carbamoylbenzamide **P171**
 carbamoyl chloride, diethyl- **D296**
 1-carbamoyl-2-phenylhydrazine **P75**
 2-carbamoylpyrazine **P348**
 Carbamult **P286**
 carbamylhydrazine hydrochloride **S22**
 1-carbamyl-2-phenylhydrazine **P75**
 carbanalate **A62**
 carbanil **P113**
D-(-)-carbanilic acid, 1-ethylcarbamoyl-, ethyl ester **C66**
 carbanilic acid, isopropyl ester **P305**
 carbanilide, *N,N'*-diethyl- **D297**
 carbanolate **C62**
 carbaryl **C63**
 Carbatene **M321**
 carbatox-60 **C63**
 Carbax **D261**

carbazide **C69**
 Carbazinc **Z19**
 carbazole **C64**
 9*H*-carbazole **C64**
 Carbazoline **C71**
 carbazotic acid **P187**
 Carbeetamide **C66**
 carbendazim **C65**
 carbendazime **C65**
 carbendazol **C65**
 Carbetamax **C66**
 carbetamide **C66**
 4-carbethoxy-1-methyl-4-phenylhexamethylenimine **E73**
 4-carbethoxyphenol **E158**
 Carbicron **D263**
 carbide 6-12 **E126**
 carbimide **C479**
 carbinamine **M154**
 carbinol **M116**
 carbitol acetate **E77**
 carbocholine **C60**
 carbocysteine **C67**
 carbodicyclohexylimide **D267**
 carbodiimide **C479**
 carbofos **M11**
 carbofuran **C68**
 carbogran **S31**
 carbohydrazide **C69**
 carbolic acid **P80**
 α -carboline **C70**
 β -carboline **C71**
 γ -carboline **C72**
 carbomethene **K8**
 carbon bichloride **T51**
 carbon bisulfide **C75**
 carbon black **C73**
 carbon bromide **C77**
 carbon dibromide dichloride **D130**
 carbon dichloride oxide **P152**
 carbon dichlorosulfide **T140**
 carbon dioxide **C74**
 carbon disulfide **C75**
 carbon fluoride **C79**
 carbon hexachloride **H38**
 carbonic acid ammonium salt **A168**
 carbonic acid, barium salt (1:1) **B9**
 carbonic acid diammonium salt **A168**
 carbonic acid, diethyl ester **D298**
 carbonic acid, disodium salt **S52**
 carbonic acid, dithallium(1+) salt **T102**
 carbonic acid, dithio-, cyclic *S,S*-(6-methyl-2,3-
 quinoxalinediyl)ester **Q11**
 carbonic acid gas **C74**
 carbonic acid, 2(or 4)-isooctyl-4,6 (or 2,6)-
 dinitrophenylmethyl ester **D506**
 carbonic acid, sodium salt **S52**
 carbonic anhydride **C74**
 carbonic dichloride **P152**
 carbonic difluoride **C80**
 carbonic dihydrazide **C69**
 carbonic oxide **C76**
 carbonimidodithioic acid, 3-pyridinyl-, butyl[4-(1,1-
 dimethylethyl)phenyl]methyl ester **B221**
 4,4'-carbonimidoylbis(*N,N*-dimethylbenzenamine) **A254**
 carbon monoxide **C76**
 carbon nitride **C482**
 carbon nitride ion **C481**
 carbonochloridic acid, butyl ester **B254**
 carbonochloridic acid, ethyl ester **E107**
 carbonochloridic acid, 1-methylethyl ester **I124**
 carbonochloridic acid, phenyl ester **P97**
 carbonothioic dichloride **T140**
 carbonothioic dihydrazide **T124**
 carbon oxide **C76**
 carbon oxide sulfide **C81**
 carbon oxychloride **P152**
 carbon oxyfluoride **C80**
 carbon oxysulfide **C81**
 carbon silicide **S31**
 carbon sulfide **C75**
 carbon tetrabromide **C77**
 carbon tetrachloride **C78**
 carbon tetrafluoride **C79**
 carbon trifluoride **T292**
 carbon triiodide **I51**
 carbonyl chloride **P152**
 carbonyl diamide **U12**
 carbonyl dichloride **P152**
 carbonyl difluoride oxide **C80**
 carbonyl fluoride **C80**
 carbonyl sulfide **C81**
 carbophenothion **C82**
 carborundum **S31**
 carbostyryl **H118**
 carbosulfan **C83**
 Carbowax **P225**
 5-carboxanilido-2,3-dihydro-6-methyl-1,4-oxathiin **C84**
 carboxin **C84**
 carboxin sulfone **O56**
 carboxyacetic acid **M17**
 2-carboxybenzanilide **P130**
 2-carboxy-4'-(dimethylamino)azobenzene **M304**
 carboxyethane **P310**
N-carboxymethyl-*N,N*-bis(methylenephosphonic
 acid)amine **G41**
S-(carboxymethyl)-*L*-cysteine **C67**
N-(carboxymethyl)glycine **I11**
 (carboxymethylthio)acetic acid **T130**
 3-[(carboxymethyl)]thioalanine **C67**
 1-carboxynaphthalene **N15**
 2-carboxynaphthalene **N16**
 9-(*o*-carboxyphenyl)-6-hydroxy-3*H*-xanthen-3-one **F51**
 4-carboxyphthalic anhydride **T299**
 6-carboxyuracil **O34**

carbozulfan **C83**
 carbromal **C85**
 Cardigin **D335**
 Cardio Green **I30**
 Cardioreg **D339**
 Cardiospan **P5**
 Carditoxin **D335**
 Caricide **D295**
 Carinex **P231**
 Carmago White **B39**
 carminic acid **C86**
 Carmoisine **C393**
 carnauba wax **C87**
 Carnebon 200 **C136**
 Carnicowax **C87**
 carob gum **L57**
 Carophyll Red **C413**
 Carotaben Plus **C413**
 α -carotene **C88**
 β,β -carotene **C89**
 β,ϵ -carotene (6'R) **C88**
 β -carotene **C89**
 $\beta\psi$ -carotene **C90**
 γ -carotene **C90**
 ψ,ψ -carotene **L65**
 β,β -carotene-4,4'-dione **C413**
 κ,κ -carotene-6,6'-dione, 3,3-dihydroxy-(3S3'5R5'R)- **C57**
 α -carotene (natural) **C88**
 Carpene **D594**
 carrageenan **C91**
 Carstab DLTPD **D365**
 cartap hydrochloride **C92**
 Cartouche **F35**
 carubinose **M30**
 carvacrol, 5-[2-(dimethylamino)ethoxy]-, acetate (ester)
T155
 Carvene **L46**
 Carvil **F12**
 (+)-carvone **C93**
 D-carvone **C93**
 D-(+)-carvone **C93**
 (S)-carvone **C93**
 (S)-(+)-carvone **C93**
 caryophyllic acid **E187**
 Carzal **F102**
 Cascade **G26**
 casinghead (natural gasoline essence) **G8**
 Casoron **D166**
 Cassella's acid F **A135**
 castor oil **C94**
 Castrix **C463**
 catechol **C95**
 catechol dimethyl ether **V18**
 caustic potash **P254**
 caustic soda **S73**
 CB-3307 **M88**
 3025 C.B. **M49**
 2-CBA **C165**
 CCH **C34**
 CCNU **L58**
 CD5550 **D206**
 CD5950 **D209**
 CDAA **A69**
 CDBM **D126**
 CDEC **S135**
 CE 6350 **E180**
 CeCeCe **C141**
 CeeNu **L58**
 Cegramine **D315**
 Cekucap **D505**
 Cekudifol **D261**
 Cekuetion **E68**
 CELA 50 **T295**
 Celacol M **M185**
 Celathion **C321**
 Celatox DP **D257**
 Celefour DP **D257**
 Cellitazol B **D95**
 Celliton Orange R **A130**
 Celliton Red Violet RN **D76**
 Cellon **T50**
 Cellosolve **E76**
 cellosolve acetate **E79**
 Celloxan **Z11**
 Celluflex **T361**
 Celluflex CEF **T350**
 Celluflex TPP **T337**
 celluloid **C96**
 cellulose **C97**
 cellulose methyleate **M185**
 cellulose methyl ether **M185**
 cellulose nitrate **C98**
 cellulose tetranitrate **C98**
 cellumeth **M185**
 celluphos 4 **T212**
 Celphos **A104**
 cement, Portland **C99**
 Centralite **D297**
 Ceiodin **P256**
 cephalixin **C100**
 Ceragum **L57**
 Ceranine HFC Liquid **P222**
 Ceraphyl 230 **D357**
 Ceratak **P7**
 Cercobin **T137**
 Cercobin methyl **T138**
 Ceresan **E143**
 Cerespan **P5**
 cerium **C101**
 Cerospray **G53**
 Certrol **I59**
 cerubidin **D23**
 cesium **C16**
 cesium-133 **C16**

cesium hydrate **C17**
 cesium hydroxide **C17**
 cesium nitrate **C18**
 Cetacourt **H95**
 cetalkonium chloride **B41**
 cetalkonium chloride **C103**
 Cetamol BMB **B248**
 Cethion **E68**
 Cetiprin **E16**
 Cetol **C103**
 cetyl alcohol **C102**
 cetyldimethylbenzylammonium chloride **C103**
 cetylpyridinium chloride **C104**
 cetyltrimethylammonium bromide **C105**
 Ceylon isinglass **A58**
 CF12 **D204**
 CFC-113 **T269**
 5243-K-CG **C212**
 CGA 17020 **D371**
 CGA 92194 **O42**
 CH 13-437 **N2**
 chalcedony **S29**
 chalk **C25**
 Challenge **G18**
 chameleon mineral **P260**
 Channing's solution **P266**
 Charge **C534**
 CHA-sulfate **C515**
 chavicol methyl ether **A75**
 1,3-CHBP **B172**
 Checkmate **S66**
 Cheetah R **F16**
 Chemagro B-1776 **T209**
 Chemaïd **S63**
 Chem-Fish **R18**
 Chemicet Yellow G **C410**
 Chemicide **C313**
 Chemit **P300**
 Chemitex **M40**
 Chemition **F11**
 Chemitte **A266**
 Chemquat 16/50 **C105**
 Chemrat **P193**
 chert **S29**
 chert **Q1**
 C,C'-(1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-en-2,3-ylene)(dimethyl sulfite) **E19**
 Chile saltpeter **S80**
 Chim **P145**
 Chimac endo **E20**
 Chimigor **D376**
 Chinese isinglass **A58**
 chinine **Q6**
 Chinizarin **Q7**
 Chinofer **I70**
 chinoleine **Q9**
 chinomethionat **Q11**
 Chinosol **H120**
 Chinothionat **T142**
 Chinyfungin **N210**
 chlomethoxyfen **C106**
 chloracetic acid, ethyl ester **E106**
 chloracetic chloride **C151**
 chloral **C107**
 chloral hydrate **C108**
 chlorallylene **A78**
 chloralose **C109**
 α-chloralose **C109**
 chloramben **C110**
 chlorambucil **C111**
 Chloramex **C114**
 chloramide **C112**
 chloramine **C112**
 Chloramine Carbon Black S **C403**
 chloramine T **C113**
 chloramphenicol **C114**
 chloranil **C115**
 o-chloraniline **C154**
 chlorate of potash **P242**
 chlorbromuron **C116**
 chlorbufam **C117**
 chlorbufame **C117**
 Chlorbutium **C111**
 chlordan **C118**
 chlordanes **C118**
 chlordecone **C119**
 chlordiazepoxide **C120**
 chlordinform **C121**
 Chlordion **C139**
 chlorendic acid **C122**
 chlorendic anhydride **C123**
 chlorethiazol **C360**
 Chlorez **C132**
 chlorfenac **C124**
 chlorfenethol **C125**
 chlorfenprop-methyl **C126**
 chlorfenson **C127**
 chlorfenvinphos **C128**
 chlorflurenol-methyl **C129**
 chlorflurenol methyl ester **C129**
 Chlorfurecol **C129**
 chlorhexidine **C130**
 chloric acid, barium salt **B10**
 chloric acid, calcium salt **C26**
 chloric acid, copper salt **C432**
 chloric acid, magnesium salt **M3**
 chloric acid, sodium salt **S53**
 chloridazon **C131**
 Chlorinat **B4**
 chlorinated C₂₂₋₂₆ alkanes **C134**
 chlorinated camphene (67-69% chlorine) **C48**
 chlorinated hydrochloric ether **D210**
 chlorinated paraffins **C132**
 chlorinated paraffins (C₁₂, 60% Cl) **C133**

chlorinated paraffins (C₂₃, 43% Cl) **C134**
 chlorinated paraffin waxes **C132**
 chlorine **C135**
 chlorine cyanide **C484**
 chlorine dioxide **C136**
 chlorine fluoride **C137**
 chlorine fluoride oxide **P53**
 chlorine iodide **I41**
 chlorine moniodide **I41**
 chlorine oxide **C136**
 chlorine(IV) oxide **C136**
 chlorine oxyfluoride **P53**
 chlorine pentafluoride **C137**
 chlorine peroxide **C136**
 chlorine trifluoride **C138**
 Chlorizyl **C312**
 chlormadinone acetate **C139**
 chlormephos **C140**
 chlormequat chloride **C141**
 chlormethine **M38**
 Chlormite **C276**
 Chlornaftina **C142**
 chlornaphazine **C142**
 α-chlornaphthalene **C217**
 Chloro **C259**
 chloroacetaldehyde **C143**
 2-chloroacetaldehyde **C143**
 chloroacetaldehyde monomer **C143**
 chloroacetamide **C144**
 2-chloroacetamide **C144**
 α-chloroacetamide **C144**
 chloroacetic acid **C145**
 α-chloroacetic acid **C145**
 chloroacetic acid chloride **C151**
 chloroacetic acid, methyl ester **M186**
 chloroacetic acid, sodium salt **S55**
 chloroacetone **C146**
 chloroacetonitrile **C147**
 2-chloroacetophenone **C148**
 4'-chloroacetophenone **C149**
 α-chloroacetophenone **C148**
 6-chloro-17-α-acetoxy-4,6-pregnadiene-3,20-dione
C139
 4-(chloroacetyl)acetanilide **C150**
 chloroacetyl chloride **C151**
 N-(chloroacetyl)-N-(2,6-diethylphenyl)glycine, ethyl ester
D282
 2-chloroacrylonitrile **C152**
 α-chloroacrylonitrile **C152**
 chloroalkanes, C10-C12 **C133**
 3-chloroallyl chloride **D250**
 γ-chloroallyl chloride **D250**
 2-chloroallyl diethyldithiocarbamate **S135**
 chloroallylene **A78**
 N-(3-chloroallyl)hexaminium chloride **C153**
 1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride
C153

chloroamine **C112**
 2-chloro-4-aminoaniline **C242**
 2-chloro-4-aminoaniline sulfate **C243**
 3-chloro-4-aminoaniline sulfate **C243**
 2-chloro-4-aminoanisole **C158**
 p-chloro-o-aminophenol **A124**
 2-chloroaniline **C154**
 3-chloroaniline **C155**
 4-chloroaniline **C156**
 m-chloroaniline **C155**
 N-chloroaniline **C157**
 o-chloroaniline **C154**
 p-chloroaniline **C156**
 3-chloroanisidine **C158**
 3-chloro-p-anisidine **C158**
 1-chloro-9,10-anthracenedione **C159**
 2-chloro-9,10-anthracenedione **C160**
 1-chloroanthraquinone **C159**
 1-chloro-9,10-anthraquinone **C159**
 2-chloroanthraquinone **C160**
 Chloroben **D188**
 2-chlorobenzaldehyde **C161**
 3-chlorobenzaldehyde **C162**
 α-chlorobenzaldehyde **B82**
 m-chlorobenzaldehyde **C162**
 o-chlorobenzaldehyde **C161**
 o-chlorobenzalmalononitrile **C175**
 2-chlorobenzenamine **C154**
 N-chlorobenzenamine **C157**
 chlorobenzene **C163**
 3-chlorobenzeneamine **C155**
 4-chlorobenzeneamine **C156**
 3-chlorobenzenecarboperoxoic acid **C237**
 o-chlorobenzenecarboxaldehyde **C161**
 2-chloro-1,4-benzenediamine **C242**
 4-chloro-1,3-benzenediamine **C244**
 2-chloro-1,4-benzenediamine sulfate **C243**
 chlorobenzilate **C164**
 2-chlorobenzoic acid **C165**
 o-chlorobenzoic acid **C165**
 6-chloro-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-
 dioxide **C287**
 2-chlorobenzotrichloride **C166**
 4-chlorobenzotrichloride **C167**
 o-chlorobenzotrichloride **C166**
 p-chlorobenzotrichloride **C167**
 2-chlorobenzotrifluoride **C168**
 3-chlorobenzotrifluoride **C169**
 4-chlorobenzotrifluoride **C170**
 m-chlorobenzotrifluoride **C169**
 o-chlorobenzotrifluoride **C168**
 p-chlorobenzotrifluoride **C170**
 5-chloro-2-benzoxazoline **Z25**
 1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indole-3-acetic
 acid **I35**
 4-chlorobenzoyl peroxide **C171**
 p-chlorobenzoyl peroxide **C171**

chlorobenzylate **C164**
 2-chlorobenzyl chloride **C172**
 3-chlorobenzyl chloride **C173**
 4-chlorobenzyl chloride **C174**
m-chlorobenzylchloride **C173**
o-chlorobenzyl chloride **C172**
p-chlorobenzyl chloride **C174**
 1-(4-chlorobenzyl)-1-cyclopentyl-3-phenylurea **P19**
 5-(4-chlorobenzyl)-*N,N*-diethylthiocarbamate **T117**
 α -(*o*-chlorobenzylidene)malonitrile **C175**
 2-chlorobenzylidenemalononitrile **C175**
 3-chloro-[1,1'-biphenyl]-4-ol **C249**
 3-chloro-4-biphenylol **C249**
 2-chloro-*N,N*-bis(2-chloroethyl)ethanamine **T349**
 1-chloro-2,2-bis(*p*-chlorophenyl)ethane **D32**
 1-chloro-2,2-bis(*p*-chlorophenyl)ethylene **D33**
 2-chloro-4,6-bis(ethylamino)-*s*-triazine **S37**
syn-chlorobromoethane **B170**
 chlorobromomethane **B171**
 1-(3-chloro-4-bromophenyl)-3-methylmethoxyurea **C116**
 ω -chlorobromopropane **B172**
 chlorobutadiene **C262**
 2-chloro-1,3-butadiene **C262**
 1-chlorobutane **B251**
 2-chlorobutane **B252**
 4-chlorobutanenitrile **C180**
 1-chloro-2-butene **C176**
 1-chloro-3-butene **C179**
 2-chlorobutene **C177**
 2-chloro-2-butene **C177**
 2-chloro-3-butene **C178**
 3-chloro-1-butene **C178**
 4-chloro-1-butene **C179**
 α -chloro- β -butylene **C176**
 γ -chloro- α -butylene **C178**
 4-chlorobut-2-ynyl **B4**
 4-chloro-2-butyryl(3-chlorophenyl)carbamate **B4**
 4-chlorobutyronitrile **C180**
 γ -chlorobutyronitrile **C180**
m-chlorocarbamic acid, isopropyl ester **C312**
 3-chlorocarbamilate **B4**
m-chlorocarbamic acid, 1-methyl-2-propynyl ester **C117**
 3-chlorochlordene **H15**
 2-chloro-*N*-(2-chloroethyl)-*N*-ethylethanamine **H82**
 1-chloro-2-(β -chloroethoxy)ethane **B120**
 2-chloro-*N*-(2-chloroethyl)-*N*-methylethanamine, *N*-oxide
M39
 1-chloro-2-(β -chloroisopropoxy)propane **D221**
 1-chloro-2-(chloromethyl)benzene **C172**
 1-chloro-3-(chloromethyl)benzene **C173**
 1-chloro-4-(chloromethyl)benzene **C174**
 3-chloro-4-(chloromethyl)-1-[3-(trifluoromethyl)phenyl]-2-
 pyrrolidone **F87**
 (3*RS*,4*RS*,5*SR*)-3-chloro-4-chloromethyl-1-(α,α,α -
 trifluoro-*m*-tolyl)-2-pyrrolidone (in ratio 3:1) **F87**
 5-chloro-*N*-(2-chloro-4-nitrophenyl)-2-hydroxybenzamide
N52
 4-chloro-*N*-(2-chloro-4-nitrophenyl)-3-(trifluoromethyl)-
 benzenesulfonamide **F91**
 4-chloro- α -(4-chlorophenyl)- α -benzenemethanol **D261**
 4-chloro- α -(4-chlorophenyl)- α -hydroxybenzene acetic acid,
 1-methylethyl ester **C276**
 4-chloro-1-(4-chlorophenylsulfonyl)benzene **B127**
 chlorocholine chloride **C141**
 chlorochromic anhydride **C339**
 chlorocresol **C183**
 3-chloro-*o*-cresol **C181**
 3-chloro-*p*-cresol **C182**
 4-chloro-*m*-cresol **C183**
 4-chloro-*o*-cresol **C184**
 5-chloro-*o*-cresol **C185**
 6-chloro-*m*-cresol **C186**
 6-chloro-*o*-cresol **C187**
p-chloro-*m*-cresol **C183**
 chlorocyan **C484**
 2-chloro-4-(1-cyano-1-methylethylamino)-6-ethylamino-
 1,3,5-triazine **C480**
 chlorocyclizine hydrochloride **C188**
 4-chloro-2-cyclopentylphenol **C189**
 7-chloro-6-demethyltetracycline **D47**
 7(*S*)-chloro-7-deoxylincomycin **C354**
 α -chloro-*N,N*-diallylacetamide **A69**
 1-chloro-2,4-diaminobenzene **C244**
 4-chloro-1,2-diaminobenzene **C245**
 1-chlorodibenzodioxin **D107**
 1-chlorodibenzo[*b,e*][1,4]dioxin **D107**
 2-chlorodibenzodioxin **D108**
 2-chlorodibenzo[*b,e*][1,4]dioxin **D108**
 chlorodibenzofuran **D112**
 chlorodibromomethane **D126**
 4-chloro-2,6-dibromophenol **D127**
 3-chloro-1,2-dibromopropane **D128**
 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethyl]benzene
D29
 (*Z*)-2-chloro-1-(2,4-dichlorophenyl)ethenyl dimethyl
 phosphate **D460**
 2-chloro-1-(2,4-dichlorophenyl)vinyl diethyl phosphate
C128
 2-chloro-1-(2,4-dichlorophenyl)vinyl dimethyl phosphate
D460
 chlorodiethoxyphosphine oxide **D299**
 3-chloro-7-diethoxyphosphinothioxy-4-methylcoumarin
C446
 3-chloro-4-diethylaminobenzenediazonium trichlorozincate
C190
 7-chloro-1-[2-(diethylamino)ethyl]-5-(2-fluorophenyl)-1,3-
 dihydro-2*H*-1,4-benzodiazepin-2-one **F84**
 6-chloro-9-[[4-(diethylamino)-1-methylbutyl]amino]-2-
 methoxyacridine **M55**
 7-chloro-4-(diethylamino-1-methylbutylamino)quinoline
C281
 2-chloro-2',6'-diethyl-*N*-(methoxymethyl)acetanilide **A60**
 2-chloro-2',6'-diethyl-*N*-methoxymethylacetanilide **A60**
 α -chloro-2',6'-diethyl-*N*-(methoxymethyl)acetanilide **A60**

N-[2-chloro-1-(diethyloxyphosphinothioylthio)-ethyl]phthalimide **D68**
 2-chloro-*N*-(2,6-diethylphenyl)-*N*-(methoxymethyl)acetamide **A60**
 6-chloro-*N,N'*-diethyl-1,3,5-triazine-2,4-diamine **S37**
 6-chloro-*N*²,*N*⁴-diethyl-1,3,5-triazine-2,4-diamine **S37**
 chlorodifluorobromomethane **B168**
 chlorodifluoroethane **C191**
 1-chloro-1,1-difluoroethane **C191**
 chlorodifluoromethane **C192**
 2-chloro-1-(difluoromethoxy)-1,1,2-trifluoroethane **E27**
 2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane **I105**
 chlorodifluoromonobromomethane **B168**
 10-chloro-5,10-dihydroarsacridine **D541**
 6-chloro-3,4-dihydro-2*H*-1,2,4-benzothiadiazine-7-sulfonamide-1,1-dioxide **H94**
S-[2-chloro-1-(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)ethyl] *O,O*-diethyl phosphorodithioate **D68**
 (*R*)-*N*-[(5-chloro-3,4-dihydro-8-hydroxy-3-methyl-1-oxo-1*H*-2-benzopyran-7-yl)carbonyl]phenylalanine **O1**
 2-chloro-5-(2,3-dihydro-1-hydroxy-3-oxo-1*H*-isoindol-1-yl)benzenesulfonamide **C318**
 7-chloro-1,3-dihydro-3-hydroxy-5-phenyl-2*H*-1,4-benzodiazepin-2-one **O48**
 7-chloro-1,3-dihydro-1-methyl-5-phenyl-2*H*-1,4-benzodiazepin-2-one **D98**
 4-chloro-2,3-dihydro-2-oxobenzothiazol-3-ylacetic acid **B27**
 5-6-chloro-2,3-dihydro-2-oxo-1,3-oxazolo[4,5-*b*]pyridin-3-ylmethyl *O,O*-dimethyl phosphorothioate **A259**
 10-chloro-5,10-dihydrophenarsazine **D541**
 4-chloro-2,5-dimethoxyaniline **C193**
 4-chloro-2,5-dimethoxybenzenamine **C193**
 7-chloro-4,6-dimethoxycoumarin-3-one-2-spiro-1'-(2'-methoxy-6'-methylcyclohex-2'-en-4'-one) **G46**
 chlorodimethoxyphosphine sulfide **D407**
 6-chloro-3-dimethoxyphosphinoylthiomethyl-1,3-oxazolo[4,5-*b*]pyridin-2(3*H*)-one **A259**
 2-chloro-4-dimethylamino-6-methylpyrimidine **C463**
 7-chloro-4-dimethylamino-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-1,11-dioxo-2-naphthacenecarboxamide **D47**
 7-chloro-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-2-**C316**
 7-chloro-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-[4*S*-(4α,4aα,5aα,6β,12aα)]-2-naphthacenecarboxamide **C316**
 2-chloro-10-(3-dimethylaminopropyl)phenothiazine **C310**
 chlorodimethyl ether **C214**
 6-chloro-*N*-(1,1-dimethylethyl)-*N'*-ethyl-1,3,5-triazine-2,4-diamine **T24**
 5-chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1*H*,3*H*)-pyrimidinedione **T20**
N'-[3-chloro-4-[5-(1,1-dimethylethyl)-2-oxo-1,3,4-oxadiazol-3(2*H*)-yl]phenyl]-*N,N*-dimethylurea **D368**
 4-chloro-3,5-dimethylphenol **C306**
 2-chloro-*N,N*-dimethyl-10*H*-phenothiazine-10-propanamine **C310**
 2-chloro-*N*-(2,6-dimethylphenyl)-*N*-(2-methoxyethyl)-acetamide **D371**
 2-chloro-4,5-dimethylphenyl methylcarbamate **C62**
 2-chloro-*N*-(2,6-dimethylphenyl)-*N*-(1*H*-pyrazol-1-ylmethyl)acetamide **M98**
 (±)-2-chloro-*N*-(2,6-dimethylphenyl)-*N*-(tetrahydro-2-oxo-3-furanyl)-acetamide **O26**
 4'-chloro-2,2-dimethylvaleraniide **M340**
 chlorodinitrobenzene **C194**
 1-chloro-2,4-dinitrobenzene **C194**
 2-chloro-1,3-dinitrobenzene **C195**
 4-chloro-1,3-dinitrobenzene **C194**
 6-chloro-1,3-dinitrobenzene **C194**
 2-chloro-*N*-[2,6-dinitro-4-(trifluoromethyl)phenyl]-*N*-ethyl-6-fluorobenzenemethanamine **F45**
 1-(*o*-chloro-α,α-diphenylbenzyl)imidazole **C365**
 chlorodiphenyl (21% Cl) **A234**
 chlorodiphenyl (32% Cl) **A235**
 chlorodiphenyl (42% Cl) **A236**
 chlorodiphenyl (48% Cl) **A237**
 2-[4-(2-chloro-1,2-diphenylethenyl)phenoxy]-*N,N*-diethylethanamine **C361**
 4-chlorodiphenyl ether **C250**
 2-[*p*-(2-chloro-1,2-diphenylvinyl)phenoxy]triethylamine **C361**
 2-chloro-*N,N*-di-2-propenylacetamide **A69**
 1-chloro-2,3-epoxypropane **E33**
 3-chloro-1,2-epoxypropane **E33**
 2-chloroethanal **C143**
 2-chloroethanamide **C144**
 chloroethane **C196**
 chloroethanoic acid **C145**
 2-chloroethanol **C197**
 2-chloro-ethanol, phosphate (3:1) **T350**
 chloroethene **V30**
 chloroethene homopolymer **P235**
 1-chloro-2-ethenylbenzene **C282**
 1-chloro-3-ethenylbenzene **C283**
 1-chloro-4-ethenylbenzene **C284**
 1,1-(chloroethenylidene)bis(4-chlorobenzene) **D33**
 Chloroethephon **E63**
 (2-chloroethoxy)carbonyl chloride **C198**
 (2-chloroethoxy)ethene **C199**
 2-chloro-*N*-ethoxymethyl-6'-ethylacet-*o*-toluidide **A14**
 2-chloro-*N*-(ethoxymethyl)-*N*-(2-ethyl-6-methylphenyl)acetamide **A14**
 2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene **O59**
 chloroethyl **C196**
 β-chloroethyl alcohol **C197**
 2-chloro-4-ethylamino-6-isopropylamino-1,3,5-triazine **A252**
 2-chloro-4-ethylamino-6-isopropylamino-*s*-triazine **A252**
 2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile **C480**

2-[[4-chloro-6-(ethylamino)-s-triazin-2-yl]amino]-2-methylpropionitrile **C480**
N-[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]glycine, ethyl ester **E12**
2-chloroethyl carbonochloridate **C198**
2-chloroethyl chlorocarbonate **C198**
3-(2-chloroethyl)-2-[(2-chloroethyl)amino] tetrahydro-2*H*-1,3,2-oxazaphosphorin-2-oxide **I3**
2-chloroethyl chloroformate **C198**
β-chloroethyl chloroformate **C198**
chloroethylcyclohexylnitrosourea **L58**
1-(2-chloroethyl)-3-cyclohexyl-1-nitrosourea **L58**
N-(2-chloroethyl)-*N'*-cyclohexyl-*N*-nitrosourea **L58**
chloroethylene **V30**
2-chloroethyl ethyl ketone **C235**
β-chloroethyl ethyl ketone **C235**
1-(2-chloroethyl)-3-(*D*-glucopyranos-2-yl)-1-nitrosourea **C307**
1,1-(2-chloroethylidene)bis(4-chlorobenzene) **D32**
α-chloroethylidene fluoride **C191**
6-chloro-*N*-2-ethyl-*N*-4-isopropyl-1,3,5-triazine-2,4-diamine **A252**
chloroethylmercury **E143**
6-(2-chloroethyl)-6-(2-methoxyethoxy)-2,5,7,10-tetraoxa-6-silaundecane **E54**
2-chloro-6'-ethyl-*N*-(2-methoxy-1-methylethyl)acet-*o*-toluidide **M323**
6-chloro-*N*-ethyl-*N'*-(1-methylethyl)-1,3,5-triazine-2,4-diamine **A252**
2-chloro-*N*-(2-ethyl-6-methylphenyl)-*N*-(2-methoxy-1-methylethyl)acetamide **M323**
5-(2-chloroethyl)-4-methylthiazole **C360**
2-(((2-chloroethyl)nitrosoamino)carbonyl)amino)-2-deoxy-*D*-glucose **C307**
2-[3-(2-chloroethyl)-3-nitrosoureido]-2-deoxy-*D*-glucopyranose **C307**
2-chloroethylphosphonic acid **E63**
β-chloroethylphosphonic acid **E63**
(2-chloroethyl)trimethylammonium chloride **C141**
β-chloroethyltrimethylammonium chloride **C141**
2-chloroethyltris(2-methoxyethoxy)silane **E54**
2-chloroethyl vinyl ether **C199**
β-chloroethyl vinyl ether **C199**
chlorofluoromethane **C200**
N-(2-chloro-6-fluorophenyl)-*N*-ethyl-α,α,α-trifluoro-2,6-dinitro-*p*-toluidine **F45**
6-[[[3-(2-chloro-6-fluorophenyl)-5-methyl-4-isoxazoly]carbonyl]amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid **F41**
3-(2-chloro-6-fluorophenyl)-5-methyl-4-isoxazoly]penicillin **F41**
(±)-2-chloro-4'-fluoro-α-(pyrimidin-5-yl)benzhydryl alcohol **N209**
chloroform **C201**
4-chloroformanilide **C202**
chloroformic acid, allyl ester **A79**
chloroformic acid isopropyl ester **I124**
chloroformic acid, phenyl ester **P97**
chloroformyl chloride **P152**
4-chloro-*N*-furfuryl-5-sulfamoylanthranilic acid **F112**
chlorohydric acid **H99**
chlorohydrin **C265**
α-chlorohydrin **C265**
1-chloro-2-hydroxybenzene **C239**
1-chloro-3-hydroxybenzene **C240**
1-chloro-4-hydroxybenzene **C241**
2-chloro-1-hydroxybenzene **C239**
3-chloro-1-hydroxybenzene **C240**
3-chloro-4-hydroxybiphenyl **C249**
4-chloro-3-hydroxybutanenitrile **C203**
5-chloro-2-hydroxydiphenylmethane **B96**
2-chloro-*N*-(hydroxymethyl)acetamide **C204**
α-chloro-*N*-(hydroxymethyl)acetamide **C204**
4-chloro-1-hydroxy-3-methylbenzene **C183**
3-chloro-7-hydroxy-4-methylcoumarin, *O,O*-diethylphosphorothioato- **C446**
(-)-*N*-[(5-chloro-8-hydroxy-3-methyl-1-oxo-7-isochromanyl)carbonyl]-3-phenylalanine **O1**
N-[[[(3*R*-5-chloro-8-hydroxy-3-methyl-1-oxo-7-isochromanyl)carbonyl]-3-phenyl-L-alanine **O1**
5-chloro-2-[(2-hydroxy-1-naphthalenyl)azo-4-methylbenzenesulfonic acid, barium salt (2:1) **D27**
2-chloro-4-hydroxynitrobenzene **C228**
2-chloro-5-(1-hydroxy-3-oxo-1-isoidolin-1-yl)benzenesulfonamide **C318**
1-chloro-2-hydroxypropane **C266**
1-chloro-3-hydroxypropane **C268**
2-chloro-1-hydroxypropene **C267**
6-chloro-3-hydroxytoluene **C183**
7-chloroindole **C205**
2-chloroisobutane **B253**
3-chloroisobutene **C216**
α-chloroisobutylene **C215**
γ-chloroisobutylene **C216**
1-chloro-2-isocyanatobenzene **C246**
1-chloro-3-isocyanatobenzene **C247**
1-chloro-4-isocyanatobenzene **C248**
2-chloro-*N*-isopropylacetanilide **P290**
α-chloro-*N*-isopropylacetanilide **P290**
1-chloroisopropyl alcohol **C266**
2-chloroisopropyl alcohol **C267**
N-(4-chloro-6-isopropylamino-1,3,5-triazin-2-yl)glycine **P283**
S-4-chloro-*N*-isopropylcarbaniloylmethyl-*O,O*-dimethylphosphorodithioate **A212**
1-chloro-2-ketopropane **C146**
chloromethane **C206**
3-chloro-4-methoxyaniline **C158**
3-chloro-4-methoxybenzenamine **C158**
2-(2-chloro-1-methoxyethoxy)phenyl methylcarbamate **C356**
1-chloro-2-methoxy-4-methylbenzene **C209**
1-chloro-4-methoxy-3-methylbenzene **C208**
2-chloro-4-methoxy-1-methylbenzene **C207**

2-chloro-*N*[[4-methoxy-6-methyl-1,3,5-triazin-2-yl]amino]carbonyl]benzenesulfonamide **C315**
 3-(3-chloro-4-methoxyphenyl)-1,1-dimethylurea **M325**
 2-chloro-4-methoxytoluene **C207**
 3-chloro-6-methoxytoluene **C208**
 4-chloro-3-methoxytoluene **C209**
 7-chloro-2-methylamino-5-phenyl-3*H*-1,4-benzodiazepine 4-oxide **C120**
 4-chloro-5-(methylamino)-2-[3-(trifluoromethyl)phenyl]-3(2*H*)-pyridazinone **N206**
 4-chloro-5-(methylamino)-2(α,α,α -trifluoro-*m*-tolyl)-3(2*H*)-pyridazinone **N206**
 2-chloro-4-methylaniline **C291**
 3-chloro-2-methylaniline **C292**
 3-chloro-4-methylaniline **C293**
 4-chloro-2-methylaniline **C294**
 5-chloro-2-methylaniline **C296**
 6-chloro-2-methylaniline **C297**
 4-chloro-2-methylaniline hydrochloride **C295**
 3-chloro-4-methylanisole **C207**
 4-chloro-2-methylanisole **C208**
 6-chloro-3-methylanisole **C209**
 2-chloro-4-methylbenzenamine **C291**
 2-chloro-6-methylbenzenamine **C297**
 3-chloro-2-methylbenzenamine **C292**
 3-chloro-4-methylbenzenamine **C293**
 4-chloro-2-methylbenzenamine **C294**
 5-chloro-2-methylbenzenamine **C296**
 (chloromethyl)benzene **B95**
 1-chloro-2-methylbenzene **C288**
 1-chloro-3-methylbenzene **C289**
 1-chloro-4-methylbenzene **C290**
 1-chloro-2-methylbut-2-ene **C210**
 1-chloro-2-methyl-2-butene **C210**
 3-chloro-2-methylbut-1-ene **C211**
 3-chloro-2-methyl-1-butene **C211**
O-(3-chloro-4-methylcoumarin-7-yl) *O,O*-diethyl phosphorothioate **C446**
 chloromethyl cyanide **C147**
S-chloromethyl *O,O*-diethyl phosphorodithioate **C140**
 chloromethyl ether **B123**
N-[4-chloro-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]glycine **P283**
 (chloromethyl)ethylene oxide **E33**
 2-chloro-1-methylethyl ether **D26**
 2-chloro-*N*-(1-methylethyl)-*N*-phenylacetamide **P290**
O-[5-chloro-1(1-methylethyl)-1*H*-1,2,4-triazol-3-yl]-*O,O*-diethyl phosphorothioic acid ester **I79**
 1,1',1''-(chloromethylidene)trisbenzene **T363**
 5-chloro-2-methyl-4-isothiazolinone **C212**
 5-chloro-2-methyl-4-isothiazolin-3-one **C212**
 5-chloro-2-methyl-4-isothiazolinone calcium chloride complex **C213**
 chloromethyl methyl ether **C214**
 1-chloro-2-methyl-3-nitrobenzene **C233**
 4-chloro-1-methyl-2-nitrobenzene **C232**
 (chloromethyl)oxirane **E33**
O-(3-chloro-4-methyl-2-oxo-2*H*-1-benzopyran-7-yl) *O,O*-diethyl phosphorothioate **C446**
O-3-chloro-4-methyl-2-oxo-2*H*-chromen-7-yl *O,O*-diethyl phosphorothioate **C446**
 2-chloro-5-methylphenol **C186**
 2-chloro-6-methylphenol **C187**
 3-chloro-2-methylphenol **C181**
 3-chloro-4-methylphenol **C182**
 3-chloro-6-methylphenol **C185**
 4-chloro-2-methylphenol **C184**
 4-chloro-3-methylphenol **C183**
 5-chloro-2-methylphenol **C185**
 6-chloro-2-methylphenol **C187**
 6-chloro-3-methylphenol **C186**
 2-chloro-5-methylphenol methyl ether **C209**
 4-chloro-2-methylphenol methyl ether **C208**
 4-chloro-2-methylphenoxyacetic acid **M32**
 4-(4-chloro-2-methylphenoxy)butanoic acid **M34**
 4-(4-chloro-2-methylphenoxy)butyric acid **M34**
 (4-chloro-2-methylphenoxy)ethanethioic acid, *S*-ethyl ester **M33**
 (\pm)-2-(4-chloro-2-methylphenoxy)propanoic acid **M40**
 7-chloro-1-methyl-5-phenyl-3*H*-1,4-benzodiazepin-2(1*H*)-one **D98**
N'-(4-chloro-2-methylphenyl)-*N,N*-dimethylmethanimidamide **C121**
 3-(3-chloro-4-methylphenyl)-1,1-dimethylurea **C298**
N'-(3-chloro-4-methylphenyl)-*N,N*-dimethylurea **C298**
 2-chloro-10-[3-(4-methyl-1-piperazinyl)propyl]-10*H*-phenothiazine **P276**
 2-chloro-2-methylpropane **B253**
 2-chloro-3-methylpropane **B252**
 1-chloro-2-methylpropene **C215**
 1-chloro-2-methyl-1-propene **C215**
 3-chloro-2-methylpropene **C216**
 3-chloro-2-methylprop-1-ene **C216**
 3-chloro-2-methyl-1-propene **C216**
 2-chloromethylpyridine hydrochloride **P186**
 (chloromethyl)trichlorosilane **T246**
 1-chloronaphthalene **C217**
 2-chloronaphthalene **C218**
 α -chloronaphthalene **C217**
 β -chloronaphthalene **C218**
 chloroneb **C219**
 2-chloro-4-nitroaniline **C220**
 4-chloro-2-nitroaniline **C221**
o-chloro-*p*-nitroaniline **C220**
p-chloro-*o*-nitroaniline **C221**
 4-chloro-2-nitrobenzenamine **C221**
 chloro-*m*-nitrobenzene **C223**
 chloro-*o*-nitrobenzene **C222**
 1-chloro-2-nitrobenzene **C222**
 1-chloro-3-nitrobenzene **C223**
 1-chloro-4-nitrobenzene **C224**
 2-chloronitrobenzene **C222**
 3-chloronitrobenzene **C223**
 4-chloronitrobenzene **C224**

4-chloro-1-nitrobenzene **C224**
m-chloronitrobenzene **C223**
o-chloronitrobenzene **C222**
p-chloronitrobenzene **C224**
 2-chloro-4-nitrobenzeneamine **C220**
 4-chloro-3-nitrobenzotrifluoride **C225**
 1-chloro-1-nitroethane **C226**
 2-chloro-4-nitrophenol **C227**
 3-chloro-4-nitrophenol **C228**
 3-chloro-6-nitrophenol **C230**
 4-chloro-2-nitrophenol **C229**
 4-chloro-*o*-nitrophenol **C229**
 5-chloro-2-nitrophenol **C230**
 2-chloro-6-nitro-3-phenoxyaniline **A32**
 2-chloro-6-nitro-3-phenoxybenzenamine **A32**
O-(3-chloro-4-nitrophenyl) *O,O*-dimethyl phosphorothioate **C320**
 1-chloro-1-nitropropane **C231**
 2-chloro-6-nitrotoluene **C233**
 4-chloro-2-nitrotoluene **C232**
 6-chloro-2-nitrotoluene **C233**
 α -chloro-4-nitrotoluene **N97**
 α -chloro-*p*-nitrotoluene **N97**
 4-chloro-3-nitro- α,α,α -trifluorotoluene **C225**
 4-chloro-2-oxo-3(2*H*)-benzothiazoleacetic acid **B27**
 4-chloro-2-oxo-3-benzothiazolineacetic acid **B27**
S-[(6-chloro-2-oxooxazolo[4,5-*b*]pyridin-3(2*H*)-yl)methyl]*O,O*-dimethyl phosphorothioate **A259**
S-6-chloro-2-oxooxazolo[4,5-*b*]pyridin-3-ylmethyl *O,O*-dimethyl phosphorothioate **A259**
 1-chloro-2-oxopropane **C146**
 4-chloro-2-oxybenzothiazolin-3-ylacetic acid **B27**
 chloropentafluoroethane **C234**
 1-chloropentane **A198**
 1-chloro-3-pentanone **C235**
 1-chloropentan-3-one **C235**
 1-chloro-4-pentanone **C236**
 5-chloro-2-pentanone **C236**
 5-chloropentan-2-one **C236**
 3-chloroperbenzoic acid **C237**
m-chloroperbenzoic acid **C237**
 3-chloroperoxybenzoic acid **C237**
 chloroperoxyl **C136**
 chlorophacinone **C238**
 chlorophenamidine **C121**
 chlorophene **B96**
 4-chlorophene-1,3-diamine **C244**
 2-chlorophenol **C239**
 3-chlorophenol **C240**
 4-chlorophenol **C241**
m-chlorophenol **C240**
o-chlorophenol **C239**
p-chlorophenol **C241**
 chlorophenothane (isomer mixture) **D35**
 4-chlorophenoxyacetic acid **C452**
p-chlorophenoxyacetic acid **C452**
 1-chloro-4-phenoxybenzene **C250**
 β -(4-chlorophenoxy)- α -(1,1-dimethylethyl)-1*H*-1,2,4-triazole-1-ethanol **T197**
 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)butan-2-ol **T197**
 2-(4-chlorophenoxy)-2-methylpropionic acid ethyl ester **C358**
 2-(*p*-chlorophenoxy)-2-methylpropionic acid, ethyl ester **C358**
 2-(3-chlorophenoxy)propanamide **C451**
 2-(*m*-chlorophenoxy)propanamide **C451**
 2-(3-chlorophenoxy)propionamide **C451**
 α -(3-chlorophenoxy)propionamide **C451**
 3-(α -*p*-chlorophenyl- β -acetyethyl)-4-hydroxycoumarin **C445**
 3-chlorophenylamine **C155**
 4-chlorophenylamine **C156**
N-[[[(4-chlorophenyl)amino]carbonyl]-2,6-difluorobenzamide **D326**
O-[4-(4-chlorophenyl)azo]phenyl]-*O,O*-dimethylphosphorothioate **A273**
O-4-(4-chlorophenylazo)phenyl *O,O*-dimethylphosphorothioate **A273**
 4-chlorophenyl benzenesulfonate **F22**
 (3-chlorophenyl)carbamic acid 4-chloro-2-butynyl ester **B4**
N-(3-chlorophenyl)carbamic acid, isopropyl ester **C312**
 (3-chlorophenyl)carbamic acid, 1-methylethyl ester **C312**
o-chlorophenylcarbonimide **C246**
 4-chlorophenyl 4-chlorobenzenesulfonate **C127**
 1-(2-chlorophenyl)-1-(4-chlorophenyl)-2,2-dichloroethane **D29**
 2-(*o*-chlorophenyl)-2-(*p*-chlorophenyl)-1,1-dichloroethane **D29**
 α -(2-chlorophenyl)- α -(4-chlorophenyl)-5-pyrimidinemethanol **F4**
 4-chloro- α -phenyl-*o*-cresol **B96**
 (4*RS*5*RS*)-5-(4-chlorophenyl)-*N*-cyclohexyl-4-methyl-2-oxo-thiazolidine-3-carboxamide **H80**
trans-5-(4-chlorophenyl)-*N*-cyclohexyl-4-methyl-2-oxo-3-thiazolidinecarboxamide **H80**
 (\pm)- α -[*N*-(3-chlorophenyl)cyclopropanecarboxamido]- γ -butyrolactone **C544**
N-(4-chlorophenyl)-*N'*-(3,4-dichlorophenyl)urea **T270**
 1-(4-chlorophenyl)-3-(2,6-difluorobenzoyl)urea **D326**
N-(4-chlorophenyl)-2,2-dimethylpentanamide **M340**
 γ -(4-chlorophenyl)-*N,N*-dimethyl-2-pyridinepropanamine, (*Z*)-2-butenedioate (1:1) **C308**
 (\pm)-3-(4-chlorophenyl)-*N,N*-dimethyl-3-(2-pyridyl)propylamine hydrogen maleate **C308**
 (*RS*)-1-(4-chlorophenyl)-4,4-dimethyl-3-(1*H*-1,2,4-triazol-1-ylmethyl)pentan-3-ol **T11**
 3-(*p*-chlorophenyl)-1,1-dimethylurea **M350**
N'-(4-chlorophenyl)-*N,N*-dimethylurea **M350**
 1-[(2-chlorophenyl)diphenylmethyl]-1*H*-imidazole **C365**
 2-chloro-1,4-phenylenediamine **C242**
 2-chloro-*p*-phenylenediamine **C242**
 4-chloro-1,2-phenylenediamine **C245**

- 4-chloro-1,3-phenylenediamine **C244**
 4-chlorophenylene-1,3-diamine **C244**
 4-chloro-*m*-phenylenediamine **C244**
 4-chloro-*o*-phenylenediamine **C245**
o-chloro-*p*-phenylenediamine **C242**
p-chloro-*m*-phenylenediamine **C244**
p-chloro-*o*-phenylenediamine **C245**
 2-chloro-1,4-phenylenediamine sulfate **C243**
 2-chloro-*p*-phenylenediamine sulfate **C243**
 1-(4-chlorophenyl)ethanone **C149**
 2-chloro-1-phenylethanone **C148**
 (±)-α-[2-(4-chlorophenyl)ethyl]-α-(1,1-dimethylethyl)-1*H*-1,2,4-triazole-1-ethanol **T11**
 (2-chlorophenyl)ethylene **C282**
 (3-chlorophenyl)ethylene **C283**
 (4-chlorophenyl)ethylene **C284**
 5-(4-chlorophenyl)-6-ethyl-2,4-pyrimidinediamine **P361**
 (±)-α-(2-chlorophenyl)-α-(4-fluorophenyl)-5-pyrimidinemethanol **N209**
N-(4-chlorophenyl)formamide **C202**
 4-(2-chlorophenylhydrazono)-3-methyl-1,2-oxazol-5-(4*H*)-one **D600**
 3-[1-(4-chlorophenyl)]-4-hydroxy-2*H*-1-benzopyran-2-one **C445**
 2-chlorophenyl isocyanate **C246**
 3-chlorophenyl isocyanate **C247**
 4-chlorophenyl isocyanate **C248**
m-chlorophenyl isocyanate **C247**
o-chlorophenyl isocyanate **C246**
p-chlorophenyl isocyanate **C248**
 3-(*p*-chlorophenyl)-1-methoxy-1-methylurea **M345**
N'-(4-chlorophenyl)-*N*-methoxy-*N*-methylurea **M345**
 2-(4-chlorophenyl)-α-methyl-5-benzoxazoleacetic acid **B34**
N-[(4-chlorophenyl)methyl]-*N*-cyclopentyl-*N'*-phenylurea **P19**
 S-[(4-chlorophenyl)methyl]diethylcarbamoithioate **T117**
 (*R**,*R*')-(±)-β-[(4-chlorophenyl)methyl]-α-(1,1-dimethylethyl)-1*H*-1,2,4-triazole-1-ethanol **P1**
 2-[(2-chlorophenyl)methyl]-4,4-dimethyl-3-isoxazolidinone **C359**
 [(2-chlorophenyl)methylene]propanedinitrile **C175**
 5-[2-[4-chlorophenyl(1-methylethyl)amino]-2-oxo-ethyl]-*O,O*-dimethylphosphorodithioate **A212**
 3-[1-(4-chlorophenyl)-3-oxobutyl]-4-hydroxycoumarin **C445**
 2-chloro-4-phenylphenol **C249**
 2-[2-(*p*-chlorophenyl)-2-phenylacetyl]indan-1,3-dione **C238**
 2-[(*p*-chlorophenyl)phenylacetyl]-1,3-indandione **C238**
 4-chlorophenyl phenyl ether **C250**
p-chlorophenyl phenyl ether **C250**
 (±)-*O*-[1-(4-chlorophenyl)-1*H*-pyrazol-4-yl] *O*-ethyl *S*-propyl phosphorothioate **P347**
 (*RS*)-[*O*-1-(4-chlorophenyl)pyrazol-4-yl] *O*-ethyl *S*-propyl phosphorothioate **P347**
 6-chloro-3-phenylpyridazin-4-yl *S*-octyl thiocarbonate **P356**
O-(6-chloro-3-phenyl-4-pyridazinyl) *S*-octyl thiocarbonate **P356**
 4-chlorophenyl sulfone **B127**
p-chlorophenyl sulfone **B127**
 1-(2-chlorophenylsulfonyl)-3-(4-methoxy-6-methyl-1,3,5-triazin-2-yl)urea **C315**
 S-[[[4-chlorophenyl]thio]methyl] *O,O*-diethyl phosphorodithioate **C82**
 1-(2-chlorophenyl)thiourea **C251**
 (2-chlorophenyl)thiourea **C251**
N-(2-chlorophenyl)thiourea **C251**
 (*o*-chlorophenyl)thiourea **C251**
 4-chlorophenyl 2,4,5-trichlorophenyl sulfide **T98**
p-chlorophenyl-2,4,5-trichlorophenyl sulfide **T98**
p-chlorophenyl 2,4,5-trichlorophenyl sulfone **T63**
 1-(4-chlorophenyl)-2,2,2-trifluoro-1-ethanone *O*-(1,3-dioxolan-2-ylmethyl)oxime **F95**
 chlorophthalidolone **C318**
 S-(2-chloro-1-phthalimidoethyl) *O,O*-diethyl phosphorodithioate **D68**
 chlorophyll **C252**
 chlorophyll a **C253**
 chlorophyll b **C254**
 chlorophyll c **C255**
 chlorophyll d **C256**
 chlorophyllin a **C257**
 chlorophyllin b **C258**
 Chloro-Pic **C259**
 chloropicrin **C259**
 1-chloropiperidine **C260**
N-chloropiperidine **C260**
 chloroplatinic acid **C261**
 chloropotassuril **P243**
 chloroprene **C262**
 β-chloroprene **C262**
 1-chloropropane **C263**
 2-chloropropane **C264**
 3-chloropropane-1,2-diol **C265**
 3-chloro-1,2-propanediol **C265**
 3-chloropropanenitrile **C274**
 (±)-2-chloropropanenitrile **C273**
 2-chloropropanoic acid, methyl ester **M189**
 1-chloro-2-propanol **C266**
 1-chloro-3-propanol **C268**
 2-chloropropanol **C267**
 2-chloro-1-propanol **C267**
 3-chloropropanol **C268**
 3-chloro-1-propanol **C268**
 1-chloro-2-propanone **C146**
 3-chloropropanonitrile **C274**
 3-chloropropanyl chloride **C275**
 1-chloroprop-2-ene **A78**
 1-chloro-2-propene **A78**
 2-chloropropene **C271**
 2-chloroprop-1-ene **C271**
 2-chloro-1-propene **C271**
 3-chloropropene **A78**

cis-1-chloropropene **C270**
cis-1-chloro-1-propene **C270**
(E)-1-chloropropene **C269**
E-1-chloro-1-propene **C269**
trans-1-chloropropene **C269**
trans-1-chloro-1-propene **C269**
(Z)-1-chloropropene **C270**
Z-1-chloro-1-propene **C270**
2-chloropropionic acid **C272**
 α -chloropropionic acid **C272**
2-chloropropionitrile **C273**
3-chloropropionitrile **C274**
 β -chloropropionitrile **C274**
3-chloropropionyl chloride **C275**
2-chloropropyl alcohol **C266**
chloropropylate **C276**
3-chloropropylene **A78**
3-chloro-1-propylene **A78**
 α -chloropropylene **A78**
3-chloropropylene glycol **C265**
chloropropylene oxide **E33**
3-chloro-1,2-propylene oxide **E33**
3-chloropropyl methyl ketone **C236**
3-chloropropyl octyl sulfoxide **C277**
3-chloropropyne **C278**
2-chloro-*N*-(pyrazol-1-ylmethyl)acet-2',6'-xylidine **M98**
2-chloropyridine **C279**
3-chloropyridine **C280**
 α -chloropyridine **C279**
m-chloropyridine **C280**
o-chloropyridine **C279**
1-[(6-chloro-3-pyridinyl)methyl]-*N*-nitro-2-imidazolidinimine **I8**
1-(6-chloro-3-pyridylmethyl)-*N*-nitroimidazolidin-2-ylideneamine **I8**
chloroquine **C281**
*N*⁴-(7-chloro-4-quinolinyl)-*N*¹,*N*¹-diethyl-1,4-pentanediamine **C281**
2-[4-[(6-chloro-2-quinoxalinyloxy]phenoxy]propanoic acid, ethyl ester **Q13**
2-chlorostyrene **C282**
3-chlorostyrene **C283**
4-chlorostyrene **C284**
m-chlorostyrene **C283**
o-chlorostyrene **C282**
p-chlorostyrene **C284**
6-chloro-7-sulfamoyl-1,2,4-benzothiadiazine 1,1-dioxide **C287**
chlorosulfonic acid **C285**
chlorosulfuric acid **C285**
chlorothalonil **C286**
chlorothiamide **C319**
chlorothiazide **C287**
2-chlorotoluene **C288**
3-chlorotoluene **C289**
4-chlorotoluene **C290**
 α -chlorotoluene **B95**
m-chlorotoluene **C289**
o-chlorotoluene **C288**
p-chlorotoluene **C290**
N-chloro-*p*-toluenesulfonamide, sodium salt **C113**
2-chloro-6-toluidine **C297**
2-chloro-*p*-toluidine **C291**
3-chloro-*o*-toluidine **C292**
3-chloro-*p*-toluidine **C293**
4-chloro-2-toluidine **C294**
4-chloro-*o*-toluidine **C294**
5-chloro-2-toluidine **C296**
5-chloro-*o*-toluidine **C296**
6-chloro-2-toluidine **C297**
6-chloro-*o*-toluidine **C297**
m-chloro-*o*-toluidine **C292**
m-chloro-*p*-toluidine **C293**
o-chloro-*p*-toluidine **C291**
p-chloro-*o*-toluidine **C294**
4-chloro-2-toluidine hydrochloride **C295**
4-chloro-*o*-toluidine hydrochloride **C295**
chlorotoluron **C298**
N'-(4-chloro-*o*-tolyl)-*N,N*-dimethylformamidine **C121**
3-(3-chloro-*p*-tolyl)-1,1-dimethylurea **C298**
(4-chloro-*o*-tolylloxy)acetic acid **M32**
4-(4-chloro-*o*-tolylloxy)butyric acid **M34**
(\pm)-2-[(4-chloro-*o*-tolyl)oxy]propionic acid **M40**
(*RS*)-2-(4-chloro-*o*-tolylloxy)propionic acid **M40**
[(4-chloro-*o*-tolyl)oxy]thioacetic acid, *S*-ethyl ester **M33**
chlorotriane **C299**
chlorotriazine **C492**
1-chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]benzene **D34**
1-chloro-2-(trichloromethyl)benzene **C166**
1-chloro-4-(trichloromethyl)benzene **C167**
2-chloro-6-(trichloromethyl)pyridine **N66**
(*Z*)-2-chloro-1-(2,4,5-trichlorophenyl)vinyl dimethyl phosphate **T60**
6-chloro-*N,N,N'*-triethyl-1,3,5-triazine-2,4-diamine **T275**
chlorotrifluoride **C138**
4'-chloro-2,2,2-trifluoroacetophenone *O*-1,3-dioxolan-2-ylmethyloxime **F95**
chloro-1,1,1-trifluoroethane **C300**
1-chloro-2,2,2-trifluoroethane **C300**
2-chloro-1,1,1-trifluoroethane **C300**
chlorotrifluoroethene **C301**
2-chloro-1,1,2-trifluoroethyl difluoromethyl ether **E27**
chlorotrifluoroethylene **C301**
1-chloro-1,2,2-trifluoroethylene **C301**
1-chloro-2,2,2-trifluoroethyl ether difluoromethyl **I105**
(*E*)-4-chloro- α,α,α -trifluoro-*N*-(1-imidazol-1-yl-2-propoxyethylidene)-*o*-toluidine **T289**
chlorotrifluoromethane **C302**
1-chloro-2-(trifluoromethyl)benzene **C168**
1-chloro-3-(trifluoromethyl)benzene **C169**
1-chloro-4-(trifluoromethyl)benzene **C170**
5-[2-chloro-4-(trifluoromethyl)phenoxy]-*N*-(methylsulfonyl)-2-nitrobenzamide **F98**

5-(2-chloro-4-(trifluoromethyl)phenoxy)-2-nitrobenzoic acid **A30**
 (E-1-[1[[4-chloro-2-(trifluoromethyl)phenyl]imino]-2-propoxyethyl]-1*H*-imidazole **T289**
 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethylcyclopropanecarboxylate **T15**
 2-chloro- α,α,α -trifluorotoluene **C168**
 3-chloro- α,α,α -trifluorotoluene **C169**
 4-chloro- α,α,α -trifluorotoluene **C170**
m-chloro- α,α,α -trifluorotoluene **C169**
o-chloro- α,α,α -trifluorotoluene **C168**
p-chloro- α,α,α -trifluorotoluene **C170**
 5-(2-chloro- α,α,α -trifluoro-*p*-tolylxy)-*N*-mesyl-2-nitrobenzene **F98**
 5-(2-chloro- α,α,α -trifluoro-*p*-tolylxy)-2-nitrobenzoic acid **A30**
 O-[5-(2-chloro- α,α,α -trifluorotolylxy)-2-nitrobenzoyl]glycolic acid, ethyl ester **F66**
 chlorotrihexylsilane **C303**
 7-chloro-2',4,6-trimethoxy-6'-methylspiro [benzofuran-2(3*H*), 1'-[2]cyclohexene]-3,4'-dione **G46**
 2-chloro-*N,N,N*-trimethylethanaminium chloride **C141**
 2-chloro-*N,N,N*-trimethyl-4-pyrimidinamine **C463**
 chlorotrimethylsilane **C304**
 chlorotrimethyl-stannane **T327**
 chlorotriphenylmethane **T363**
 chlorotriphenylsilane **C305**
 (chlorotriptyl)imidazole **C365**
 chlorous acid, calcium salt **C27**
 chlorous acid, sodium salt **S54**
 chlorovinylarsine dichloride **L41**
 Chlorowax **C259**
 Chlorowax **C132**
 chloroxylam **C62**
 chloroxyleneol **C306**
 4-chloro-3,5-xyleneol **C306**
p-chloro-*m*-xyleneol **C306**
 (\pm)-(α)-2-chloro-*N*-2,6-xylylacetamido- γ -butyrolactone **O26**
 6-chloro-3,4-xylyl methylcarbamate **C62**
 Chlorozon **P11**
 chlorozotocin **C307**
 chlorphenacome **C238**
 chlorpheniramine maleate **C308**
 chlorphonium chloride **C309**
 Chlor-O-Pic **C259**
 chlorpromazine **C310**
 chlorpropamide **C311**
 chlorpropham **C312**
 chlorpyrifos **C313**
 chlorpyrifos-methyl **C314**
 chlorsulfuron **C315**
 7-chlortetracycline **C316**
 chlorthal-dimethyl **C317**
 chlorthalidone **C318**
 chlorthiamid **C319**
 chlorthiamide **C319**

chlorthion **C320**
 chlorthiophos **C321**
 Chlortocide **C298**
 Chlortox **C118**
 Chlor-Trimeton **C308**
 chlorvescent **P243**
 chlorylen **T249**
 Chlotride **C287**
 chlozolate **C322**
 cholecalciferol **C323**
 cholest-5-en-3- β -ol **C324**
 cholest-5-en-3- β -ol 4-[bis(2-chloroethyl)amino]benzeneacetate **P65**
 cholesterol **C324**
 cholesterol alcohol **C324**
 cholestrin **C324**
 cholestyramine **C325**
 cholestyramine resin **C325**
 choline **C326**
 choline chloride carbamate **C60**
 choline dichloride **C141**
 choline ion **C326**
 choline salicylate **C327**
 choline salicylate B **C327**
 choline salicylic acid salt **C327**
 Chopper **I6**
 Chormanimophene **C111**
 (*o*-choroanilino)dichlorotriazine **A208**
 Chorus **F39**
 Christensenite **T274**
 Chroman **X7**
 chromatin B **C338**
 chrome **C329**
 Chrome Leather Black EM **C403**
 Chrome Leather Blue 2B **C404**
 Chrometrace (hexahydrate) **C334**
 chrome yellow **L16**
 chromic acetate **C332**
 chromic acid **C328**
 chromic acid, calcium salt (1:1) **C28**
 chromic acid, di-*tert*-butyl ester **B255**
 chromic acid (H₂CrO₄), bis(1,1-dimethylethyl) ester **B255**
 chromic acid (H₂Cr₂O₇), disodium salt **S61**
 chromic acid (H₂Cr₂O₇), disodium salt, dihydrate **S62**
 chromic acid (H₂CrO₄), lead(2+) salt(I:I) **L16**
 chromic acid (H₂CrO₄), strontium salt (1:1) **S122**
 chromic acid, sodium salt **S56**
 chromic acid, zinc salt (1) **Z7**
 chromic anhydride **C337**
 chromic chloride **C334**
 chromic fluoride **C335**
 chromic nitrate **C336**
 chromic oxychloride **C339**
 chromic sulfate **C338**
 chromic trioxide **C337**
 chromium **C329**

chromium(3+) **C330**
 chromium(6+) **C331**
 chromium(III) **C330**
 chromium(VI) **C331**
 chromium(III) acetate **C332**
 chromium(II) chloride **C333**
 chromium(III) chloride **C334**
 chromium(VI) dioxychloride **C339**
 chromium(III) fluoride **C335**
 chromium metal **C329**
 chromium(III) nitrate **C336**
 chromium(VI) oxide **C337**
 chromium oxychloride **C339**
 chromium sodium oxide **S56**
 chromium sodium oxide **S61**
 chromium(III) sulfate **C338**
 chromium triacetate **C332**
 chromium trioxide **C337**
 chromium zinc oxide **Z7**
 chromocor **F36**
 Chromosal **C338**
 Chromotrichia factor **A117**
 chromous chloride **C333**
 chromyl chloride **C339**
Chrysanthemum cinerariaefolium chrysanthemates **P354**
N-(chrysanthemoxymethyl)-1-cyclohexene-1,2-dicarboximide **T85**
 chrysanthemummonocarboxylic acid, 3-allyl-2-methyl-4-oxo-2-cyclopenten-1-one **A68**
 chrysanthemummonocarboxylic acid, pyrethrolone ester **P352**
 chrysazin **D22**
 chrysene **C340**
 chrysofluorene **B60**
 chrysogen **N6**
 chrysoidin **C341**
 Chrysoidine **C341**
 chrysotile **C342**
 chrysotile asbestos **C342**
 CHS **C515**
 Chyaron **R4**
 CI 77180 **C2**
 Ciba 9491 **I50**
 Cibacete Diazo Navy Blue 2B **D95**
 Ciba-Geigy A 12223 **I79**
 Cibanaphthol RF **N19**
 CIBA 13437 Su **N2**
 Ciclisin **L66**
 Cidal **S5**
 Cidalina **F24**
 Cidex **G21**
 cidolysal **L66**
 Cidorel **N209**
 Cikloherb **C498**
 cincholepidine **M299**
 cineole **C343**
 1,8-cineole **C343**
 cinerin I **C344**
 cinerin II **C345**
 cinnamal **C346**
 cinnamaldehyde **C346**
 cinnamene **S126**
 cinnamic aldehyde **C346**
 cinnamyl alcohol anthranilate **C347**
 cinnamyl alcohol, formate **C348**
 cinnamyl alcohol, propionate **C349**
 cinnamyl 2-aminobenzoate **C347**
 cinnamyl *o*-aminobenzoate **C347**
 cinnamyl anthranilate **C347**
 cinnamyl formate **C348**
 cinnamyl methanoate **C348**
 cinnamyl propionate **C349**
 Cinnanizin **C358**
 Ciodrin **M167**
 Cipotril **I59**
 Cirantin **H30**
 Cire de Carnauba Poudre **C87**
 (1*R*,*cisS*) and (1*S*,*cisR*) enantiomeric isomer pair of α -cyano-3-phenoxybenzyl-3-(2, 2-dichlorovinyl)-2,2-dimethylcyclopropane carboxylate **C543**
 cislin **D46**
 cisplatin **C350**
 Citadel **F39**
 Citation **C545**
 citexal **M119**
 citral **C351**
 Citramin **B240**
 Citrashine **I4**
 Citrazon **B81**
 citric acid **C352**
 citric acid, triethyl ester **T279**
 citrinin **C353**
 Citro **C352**
 Citroflex 2 **T279**
 Citrofol A1 **T279**
 Citron Yellow **Z7**
 Citrus Red 2 **C423**
 Clarifloc **C91**
 Clarosan **T25**
 clavacin **P16**
 claviformin **P16**
 Claymore **I6**
 Clementgros **D257**
 Cleocin **C354**
 1,6-Cleve's acid **A133**
 1,7-Cleve's acid **A136**
 clindamycin **C354**
 Clinestrol **S117**
 clivorine **C355**
 Cloca **E19**
 cloethocarb **C356**
 clofentezine **C357**
 clofibrate **C358**
 clomazone **C359**

clomethiazole **C360**
 Clomid **C361**
 clomiphene citrate **C361**
 clomiphene dihydrogen citrate **C361**
 clonitralid **C362**
 Cloparin **C132**
 Cloparol **C132**
 clopidol **C363**
 Clopindol **C363**
 clopyralid **C364**
 Clor **C238**
 clotrimazole **C365**
 CMP **P77**
 CMPP **M40**
 CN **C148**
 coal naphtha **B47**
 coal tar **C366**
 coal tar extract **C366**
 coal tar oil **C453**
 coal tar pitch **C366**
 coal tar pitch volatiles **C367**
 coal tar volatiles (benzene-soluble) **C367**
 Coapt **M196**
 cobalamin **C368**
 cobalt **C369**
 cobalt black **C376**
 cobalt(II) bromide **C370**
 cobalt(II) bromide **C370**
 cobalt carbonyl **C371**
 cobalt chloride **C372**
 cobalt(II) chloride **C372**
 cobalt dibromide **C370**
 cobalt dichloride **C372**
 cobalt(II) formate **C373**
 cobalt hydrocarbonyl **C374**
 cobalt monooxide **C376**
 cobalt monosulfate **C379**
 cobalt monosulfide **C380**
 cobalt naphthoate **C375**
 cobaltous bromide **C370**
 cobaltous chloride **C372**
 cobaltous formate **C373**
 cobaltous oxide **C376**
 cobaltous sulfamate **C378**
 cobaltous sulfate **C379**
 cobaltous sulfide **C380**
 cobalt oxide **C376**
 cobalt(II) oxide **C376**
 cobalt(II) oxide **C376**
 cobalt resinate **C377**
 cobalt resinate, precipitated **C377**
 cobalt(II) sulfamate **C378**
 cobalt sulfate **C379**
 cobalt sulfate (1:1) **C379**
 cobalt(II) sulfate **C379**
 cobalt sulfide **C380**
 cobalt(II) sulfide **C380**

cobalt tetracarbonyl dimer **C371**
 Co bastab **C368**
 Cobex **D466**
 Cobratec TT100 **M164**
 cocamide DEA **C381**
 Coccidine **D465**
 Coccidot **D465**
 Coccine **C394**
 Cocculin **P188**
 cochineal **C382**
 Cochineal Red A **C394**
 cochineal solution **C382**
 cochineal tincture **C382**
 codeine phosphate **C383**
 Codelcortone **P269**
 codethyline **E151**
 coenzyme R **B112**
 Cofol **B142**
 Cogilor Rouge 319.11 **C393**
 Cohydrin **D344**
 coking tar **C366**
 colchicine **C384**
 7- α -H-colchicine **C384**
 Colchisol **C384**
 Colcin **C384**
 Colep **N137**
 Coleytl **C60**
 Collarin **P305**
 colloidal arsenic **A240**
 colloidal selenium **S14**
 COLO Acid Orange **C391**
 COLO Acid Orange G **C392**
 COLO Acid Red AV **C397**
 Cologel **M185**
 colonial spirit **M116**
 COLO Pigment Scarlet RN **C416**
 Colo-Pleon **S140**
 C.I. 10305 **P187**
 C.I. 10360 **D550**
 C.I. 10385 **C390**
 C.I. 11000 **A114**
 C.I. 11020 **M320**
 C.I. 11160 **C424**
 C.I. 11270 **C341**
 C.I. 11855 **C410**
 C.I. 12055 **C426**
 C.I. 12100 **O27**
 C.I. 12120 **C416**
 C.I. 12140 **C420**
 C.I. 12156 **C423**
 C.I. 12355 **C417**
 C.I. 13020 **M304**
 C.I. 13025 **M271**
 C.I. 14720 **C393**
 C.I. 15510 **C391**
 C.I. 15620 **C397**
 C.I. 15865:2 **C418**

C.I. 15985 **C415**
 C.I. 16150 **C395**
 C.I. 16155 **C414**
 C.I. 16230 **C392**
 C.I. 16255 **C394**
 C.I. 21090 **D96**
 C.I. 21100 **C419**
 C.I. 22610 **C404**
 C.I. 23060 **D192**
 C.I. 23630 **C408**
 C.I. 23635 **C398**
 C.I. 23860 **E190**
 C.I. 24400 **C405**
 C.I. 24401 **C406**
 C.I. 26100 **C422**
 C.I. 30145 **C407**
 C.I. 30235 **C403**
 C.I. 37010 **D180**
 C.I. 37020 **D240**
 C.I. 37025 **N74**
 C.I. 37030 **N75**
 C.I. 37035 **N76**
 C.I. 37077 **T185**
 C.I. 37100 **M259**
 C.I. 37105 **M260**
 C.I. 37107 **T187**
 C.I. 37110 **M261**
 C.I. 37125 **M141**
 C.I. 37130 **M142**
 C.I. 37230 **T172**
 C.I. 37500 **N18**
 C.I. 37505 **N19**
 C.I. 406 **O62**
 C.I. 40850 **C413**
 C.I. 42000 **M9**
 C.I. 42040 **C400**
 C.I. 42045 **C386**
 C.I. 42053 **C412**
 C.I. 42085 **C388**
 C.I. 42090 **C387**
 C.I. 42090 **C411**
 C.I. 42500 **C402**
 C.I. 44090 **C389**
 C.I. 45100 **C396**
 C.I. 45160 **C401**
 C.I. 45170 **R9**
 C.I. 45350 **C399**
 C.I. 453501 **F51**
 C.I. 45380 **E29**
 C.I. 47000 **C427**
 C.I. 47005 **Q10**
 C.I. 473 **M42**
 C.I. 50040 **N42**
 C.I. 50200 **P82**
 C.I. 50420 **C385**
 C.I. 52915 **M216**
 C.I. 58050 **Q7**

C.I. 59100 **C428**
 C.I. 60700 **A130**
 C.I. 61100 **D76**
 C.I. 64500 **C409**
 C.I. 73000 **I25**
 C.I. 73015 **I26**
 C.I. 74160 **P176**
 C.I. 75125 **L65**
 C.I. 75300 **C478**
 C.I. 75440 **E18**
 C.I. 75470 **C86**
 C.I. 75610 **G9**
 C.I. 75670 **Q2**
 C.I. 75730 **R22**
 C.I. 75781 **I26**
 C.I. 76000 **A209**
 C.I. 76010 **P102**
 C.I. 76020 **N134**
 C.I. 76043 **T174**
 C.I. 76061 **P105**
 C.I. 76070 **N133**
 C.I. 76075 **D448**
 C.I. 76515 **P363**
 C.I. 76525 **A124**
 C.I. 77000 **A96**
 C.I. 77052 **A227**
 C.I. 77085 **A242**
 C.I. 77099 **B9**
 C.I. 77185 **C3**
 C.I. 77199 **C14**
 C.I. 77322 **C376**
 C.I. 77410 **P15**
 C.I. 77491 **I74**
 C.I. 77575 **L11**
 C.I. 77580 **L19**
 C.I. 77610 **L17**
 C.I. 77613 **L24**
 C.I. 77622 **L27**
 C.I. 77630 **L30**
 C.I. 77640 **L31**
 C.I. 77755 **P260**
 C.I. 77760 **M82**
 C.I. 77764 **M70**
 C.I. 77795 **P212**
 C.I. 77805 **S14**
 C.I. 77820 **S33**
 C.I. 77860 **T158**
 C.I. 77864 **T159**
 C.I. 77891 **T165**
 C.I. 77938 **V12**
 C.I. 77940 **V16**
 C.I. 77947 **Z12**
 C.I. 77950 **Z5**
 C.I. 77955 **Z7**
 C.I. Acid Black 2 **C385**
 C.I. Acid Blue 1 **C386**
 C.I. Acid Blue 9 **C387**

C.I. Acid Blue 9, disodium salt **C411**
 C.I. Acid Dye **C414**
 C.I. Acid Green 3 **C388**
 C.I. Acid Green 50 **C389**
 C.I. Acid Orange 10 **C392**
 C.I. Acid Orange 3 **C390**
 C.I. Acid Orange 52 **M271**
 C.I. Acid Orange 7 **C391**
 C.I. Acid Red 114 **C398**
 C.I. Acid Red 14 **C393**
 C.I. Acid Red 18 **C394**
 C.I. Acid Red 2 **M304**
 C.I. Acid Red 26 **C395**
 C.I. Acid Red 27 **A108**
 C.I. Acid Red 52 **C396**
 C.I. Acid Red 88 **C397**
 C.I. Acid Violet 49 **B101**
 C.I. Acid Yellow 3 **Q10**
 C.I. Acid Yellow 73 **C399**
 C.I. Acid Yellow 73 **F51**
 C.I. Azoic Brown 29 (component) **T185**
 C.I. Azoic Coupling Component 107 **T187**
 C.I. Azoic Diazo Component 113 **T172**
 C.I. azoic diazo component 12 **M260**
 C.I. 46005B **C421**
 C.I. Basic Blue 9 **M216**
 C.I. Basic Green 1 **C400**
 C.I. Basic Green 4 **M9**
 C.I. Basic Red 1 **C401**
 C.I. Basic Red 5 **N42**
 C.I. Basic Red 9 **C402**
 C.I. Basic Red 9 monohydrochloride **C402**
 C.I. Basic Violet 10 **R9**
 C.I. Basic Violet 14 monohydrochloride **M1**
 C.I. Developer 1 **P121**
 C.I. Developer 11 **P101**
 C.I. Developer 15 **P128**
 C.I. Direct Black 38 **C403**
 C.I. Direct Blue **T366**
 C.I. Direct Blue 15 **C405**
 C.I. Direct Blue 218 **C406**
 C.I. Direct Blue 53 **E190**
 C.I. Direct Blue 6 **C404**
 C.I. Direct Blue 15, tetrasodium salt **C405**
 C.I. Direct Brown 95 **C407**
 C.I. Direct Red 39 **C408**
 C.I. Disperse Black 6 **D95**
 C.I. Disperse Blue 1 **C409**
 C.I. Disperse Yellow 3 **C410**
 C.I. Food Blue **C386**
 C.I. Food Blue 2 **C411**
 C.I. Food Green 3 **C412**
 C.I. Food Orange 8 **C413**
 C.I. Food Red 15 **R9**
 C.I. Food Red 3 **C393**
 C.I. Food Red 5 **C395**
 C.I. Food Red 6 **C414**

C.I. Food Red 7 **C394**
 C.I. Food Red 9 **A108**
 C.I. Food Yellow **Q10**
 C.I. Food Yellow 3 **C415**
 C.I. Natural Red 1 **Q2**
 C.I. Natural Red 33 **B25**
 C.I. Natural Red 4 **C86**
 C.I. Natural White 1 **G50**
 C.I. Natural Yellow **C478**
 C.I. Natural Yellow 10 & 13 **Q2**
 C.I. Natural Yellow 27 **L65**
 C.I. Oxidation Base **A209**
 C.I. Oxidation Base 16 **P102**
 C.I. Oxidation base 18 **A124**
 C.I. oxidation base 32 **P363**
 C.I. oxidation base 4 **T174**
 C.I. Pigment Black 13 **C376**
 C.I. Pigment Blue 15 **P176**
 C.I. Pigment Green 21 **P15**
 C.I. pigment metal 4 **L11**
 C.I. pigment metal 5 **T158**
 C.I. Pigment Red **I74**
 C.I. Pigment Red 23 **C417**
 C.I. Pigment Red 3 **C416**
 C.I. Pigment Red 48:2 **C418**
 C.I. Pigment Red 53, barium salt (2:1) **D27**
 C.I. Pigment White 10 **B9**
 C.I. Pigment White 11 **A227**
 C.I. Pigment White 3 **L30**
 C.I. pigment white 4 **Z12**
 C.I. Pigment White 6 **T165**
 C.I. Pigment Yellow 12 **D96**
 C.I. Pigment Yellow 13 **C419**
 C.I. Pigment Yellow 32 **S122**
 C.I. Pigment Yellow 36 **Z7**
 C.I. Pigment Yellow 48 **L17**
 C.I. Solvent Orange 15 **C421**
 C.I. Solvent Orange 2 **O27**
 C.I. Solvent Orange 7 **C420**
 C.I. Solvent Red 23 **C422**
 C.I. Solvent Red 80 **C423**
 C.I. Solvent Yellow 1 **A114**
 C.I. Solvent Yellow 14 **C426**
 C.I. Solvent Yellow 2 **M320**
 C.I. Solvent Yellow 3 **C424**
 C.I. Solvent Yellow 33 **C427**
 C.I. Solvent Yellow 34 **A254**
 C.I. Solvent Yellow 7 **C425**
 C.I. Solvent Yellow 77 **C410**
 C.I. Solvent Yellow 94 **F51**
 C.I. Vat Yellow **C428**
 C.I. Vat Yellow 4 **C428**
 Colrex Compound **C383**
 Colt **D259**
 Coltonex **F47**
 columbium **N61**
 Comac **B142**

Combat **H86**
 Combinex **P56**
 Comite **P300**
 Commando **F35**
 Commodore **C534**
 Compactrol **C44**
 Compete **F66**
 Complemix **D583**
 Comply **F17**
 Compo Rosenspray **D593**
 Compo Rosen-Spray **B137**
 Compound 469 **I105**
 Compound 711 **I101**
 Compound 864 **I16**
 compound F-2 **Z1**
 Compound 88R **A232**
 Concep II **O42**
 Concep III **F95**
 Concord **C543**
 Condore **C106**
 Condylon **C384**
 condy's crystals **P260**
 confectioner's sugar **S131**
 Confidor **I8**
 Congo Blue **T366**
 Conorid **N205**
 Contaf **H43**
 Contain **I6**
 Contimet 30 **T164**
 contraven **T22**
 Contrax-P **P193**
 Controvlor **N207**
 Convulex **S100**
 COP1 **I56**
 copper **C429**
 copper acetate **C430**
 copper acetate arsenite **C431**
 copper acetoarsenite **C431**
 copper(II) acetoarsenite **C431**
 copper-airborne **C429**
 copper bichloride **C434**
 copper bronze **C429**
 copper chlorate **C432**
 copper(II) chlorate **C432**
 copper chloride **C434**
 copper(I) chloride **C433**
 copper(II) chloride **C434**
 copper chloride oxide **C441**
 copper(II) chloride oxide hydrate **C441**
 copper(I) cyanide **C435**
 copper diacetate **C430**
 copper dinitrate **C438**
 copper EDTA **C436**
 copper 8-hydroxyquinolate **O50**
 copper-milled **C429**
 copper monochloride **C433**
 copper naphthenate **C437**

copper nitrate **C438**
 copper oxalate **C439**
 copper(I) oxide **C440**
 copper oxinate **O50**
 copper oxine **O50**
 copper oxychloride **C441**
 copper phthalocyanine **P176**
 copper suboxide **C440**
 copper sulfate **C442**
 copper(II) sulfate **C442**
 copper sulfate, ammoniated **C443**
 copper tartrate **C444**
 copper uversol **C437**
 Coragoxine **D339**
 Co-Ral **C446**
 Corasil **D257**
 Coratop **P365**
 Coraza **D540**
 Corbel **F20**
 cordycepic acid **M28**
 Coretal **O52**
 Corflex 440 **D354**
 Corflex DOA **D514**
 Cornicide **E40**
 Cornox CWK **B27**
 corn starch **S110**
 Corodane **C118**
 Corona **P360**
 Corotran **C127**
 Corozate **Z19**
 corpus luteum hormone **P282**
 corrosive sublimate **M71**
 Corticreme **H95**
 Cortilan **C313**
 cortisol **H95**
 Δ^1 -cortisol **P269**
 Corylon **M31**
 Corylone **M31**
 Coryrine **Y1**
 Cosan **S149**
 Coslan **M42**
 Cosmetol **C94**
 Cossack **F35**
 Coteran **F47**
 Cotinazin **I109**
 Cotnion-methyl **A264**
 Cotoguard **F47**
 Cotoran **F47**
 coumachlor **C445**
 Coumadin sodium **W3**
 coumafen **W1**
 Coumafuryl **F116**
 coumaphos **C446**
 coumarin **C447**
cis-o-coumarinic acid lactone **C447**
 coumarinic anhydride **C447**
 coumarone **B61**

coumatetralyl **C448**
 coumestrol **C449**
 coumithoate **C450**
 counter **T22**
 covol **P234**
 Coyden **C363**
 Coyden 25 **C363**
 CP **N66**
 CP-41845 **G41**
 CP 23426 **T198**
 CP25 **T173**
 CP3438 **T122**
 4-CP **C452**
 CP40294 **N137**
 CP 4742 **S135**
 3-CPA **C451**
 4-CPA **C452**
 CPC **C104**
 Cpiron **I72**
 CPS034 **D373**
 cratone **F124**
 Cremart **B198**
 creosote **C453**
 3-cresidine **C454**
m-cresidine **C454**
p-cresidine **C455**
 cresol **C456**
 2-cresol **C458**
 3-cresol **C457**
 4-cresol **C459**
m-cresol **C457**
o-cresol **C458**
p-cresol **C459**
p-cresol, 2,6-di-*tert*-butyl- **B245**
 cresol glycidyl ether **C460**
p-cresol methyl ether **M157**
 Creson **G47**
 Crestomycin **N38**
 cresyl glycidyl ether **C460**
 2-cresyl glycidyl ether **C461**
 4-cresyl glycidyl ether **C462**
o-cresyl glycidyl ether **C461**
p-cresyl glycidyl ether **C462**
 cresylic acid **C456**
m-cresylic acid **C457**
o-cresylic acid **C458**
p-cresylic acid **C459**
o-cresyl phosphate **T362**
 Crill 7 **P228**
 crimidine **C463**
 Crinone **P282**
 Crisodrin **M343**
 Crisquat **P11**
 cristerone T **T38**
 cristobalite **C464**
 crithminic acid **T183**
 crocidolite **C465**

Crodamine 1.18D **S111**
 Crodamol DOA **D514**
 Croderol **G25**
 Crodamol DA **D357**
 cromaril **F36**
 Cromoglycate **S57**
 Cromolyn sodium **S57**
 Croneton **E67**
 Crotex **F40**
 Crotex Steel **C145**
 Crossential L99 **L49**
 Crotamitex **C466**
 crotamiton **C466**
 α -crotin acid **C468**
 α,β -crotolactone **F124**
 γ -crotolactone **F124**
 crotonaldehyde **C467**
 crotonic acid **C468**
 α -crotonic acid, ethyl ester **E109**
E-crotonic acid, ethyl ester **E109**
 crotonic acid, 3-hydroxy-, isopropyl ester, *O*-ester with *O*-methyl *N*-ethyl phosphoramidothioate, (*E*)- **P304**
 crotonic acid, 3-hydroxy-, α -methylbenzyl ester, dimethyl phosphate, (*E*)- **M167**
 crotonic acid, 3-methyl-2-*sec*-butyl-4,6-dinitrophenyl ester **B111**
 crotonic aldehyde **C467**
 crotonyl alcohol **C470**
 crotonylene **C469**
 Crotoxypnos **M167**
 crotyl alcohol **C470**
trans-crotyl alcohol **B218**
 crotyl chloride **C176**
 Croysulfone **S146**
 crude arsenic **A244**
 crufomate **C471**
 crustecdysone **E1**
 cryolite **C472**
 cryptohalite **A174**
 crystalline: silica sand **S29**
 crystallised verdigris **C430**
 Crystodigin **D335**
 crystosol **M333**
 CS **C175**
 C-Sn-9 **T219**
 cubic nitrate **S80**
 Cudgel **F99**
 cufraneb **C473**
 Culminal MC **M185**
 Cuman **Z19**
 cumene **C474**
 ψ -cumene **T307**
 cumene hydroperoxide **C475**
 α -cumene hydroperoxide **C475**
 cumene peroxide **D264**
p-cumenol **I130**
m-cumenol methylcarbamate **I131**

3-*p*-cumenyl-1,1-dimethylurea **I133**
 cumenyl hydroperoxide **C475**
m-cumenyl methylcarbamate **I131**
o-cumenyl methylcarbamate **I116**
 cumic aldehyde **I122**
ψ-cumidine **T304**
 Cumirat **C448**
 cumoestrol **C449**
 cumol **C474**
 cumostrol **C449**
 α-cumyl alcohol **P131**
 7-cumyl hydroperoxide **C475**
 α-cumyl hydroperoxide **C475**
 cupferron **C476**
 cuprate(4-), (μ-((3,3'-((3,3'-dihydroxy(1,1'-biphenyl)-4,4'-diyl)bis(azo)bis(5-amino-4-hydroxy-2,7-naphthalenedisulfonate))(8-)))di-, tetrasodium **C406**
 cuprate(2-), [5-[4'-[[2,6-dihydroxy-3-[(2-hydroxy-5-sulfophenyl)azo]phenyl]azo][1,1'-biphenyl]-4-yl]azo-2-hydroxybenzoato, (4-)]-, disodium **C407**
 cupric acetate **C430**
 cupric acetoarsenite **P15**
 cupric chloride **C434**
 cupricin **C435**
 cupric nitrate **C438**
 cupric oxalate **C439**
 cupric oxide chloride **C441**
 cupric 8-quinolinoxide **O50**
 cupric sulfate **C442**
 cupric tartrate **C444**
 Cupridan **C440**
 cupriethylenediamine **C477**
 Cuprix **B142**
 Cuprocal **B142**
 cuprous chloride **C433**
 cuprous cyanide **C435**
 cuprous oxide **C440**
 Cuprox **C440**
 Curalan **V23**
 Curbiset **C129**
 curcumin **C478**
 Curetard **N176**
 Curetard **N155**
 Curital **D260**
 Curithane C126 **D192**
 curling factor **G46**
 Curol **F4**
 Curzate **C541**
 Cutless **F89**
 C05 (vinyl polymer) **P234**
 CVMP **T60**
 Cyaforce **H86**
 cyanamide **C479**
 cyanamide, calcium salt (1:1) **C29**
 cyanater **T22**
 cyanazine **C480**
 Cyan Blue BNC **P176**
 Cyangas **C30**
 cyanide **C481**
 cyanide anion **C481**
 cyanoacetoneitrile **M18**
 cyanoamine **C479**
 cyanobenzene **B68**
 4-cyanobenzonitrile **T27**
 cyanobromide **C483**
 cyanocobalamin **C368**
 cyanoethane **P312**
 cyanoethylene **A43**
 cyano(4-fluoro-3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate **C533**
 cyanogen **C482**
 cyanogen bromide **C483**
 cyanogen chloride **C484**
 cyanogen iodide **C485**
 cyanogen nitride **C479**
 cyanogran **S58**
 (cyanoguanidinato-*N'*)methylmercury **M251**
 cyanolyt **M196**
 cyanomethane **A20**
 1-(2-cyano-2-methoxyiminoacetyl)-3-ethylurea **C541**
N-(cyanomethyl)dimethylamine **D385**
 3-(cyanomethyl)indole **I33**
 2-cyanonitrobenzene **N90**
 3-cyanonitrobenzene **N91**
 4-cyanonitrobenzene **N92**
N-cyano-*N*-nitrosoethylamine **E157**
 1-cyanooctane **O21**
 (S)-α-cyano-3-phenoxybenzyl-(S)-2-(4-chlorophenyl)isovalerate **E49**
 α-cyano-3-phenoxybenzyl-2-(4-chlorophenyl)-3-methylbutyrate **F28**
 (RS)-α-cyano-3-phenoxybenzyl-*N*-(2-chloro-α,α,α-trifluoro-*p*-tolyl) D-valinate **F94**
 (S)-α-cyano-3-phenoxybenzyl (1*R*)-*cis*-3-(2,2-dibromovinyl)-2,2-dimethylcyclopropanecarboxylate **D46**
 RS-α-cyano-3-phenoxybenzyl (1*RS*,3*RS*;1*RS*,3*SR*)-3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate **C542**
 (S)-α-cyano-3-phenoxybenzyl (1*R*,3*S*)-2,2-dimethyl-3-[(*RS*)-1,2,2,2-tetrabromoethyl]cyclopropanecarboxylate **T194**
 cyano(3-phenoxyphenyl)methyl-4-chloro-α-(1-methylethyl)benzeneacetate **F28**
 [S-(*R,R*)]-cyano(3-phenoxyphenyl) methyl 4-chloro-α-(1-methylethyl)-, benzeneacetate **E49**
 cyano(3-phenoxyphenyl)methyl-*N*-[2-chloro-4-(trifluoromethyl)phenyl] D-valinate **F94**
 [1*R*-[1α(*S**)3α]]-cyano(3-phenoxyphenyl)methyl 3-(2,2-dibromoethenyl)-2,2-dimethylcyclopropanecarboxylate **D46**
 (1α(*S*),3α)-(+)-cyano(3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropane carboxylate **C543**

- (±)-cyano-(3-phenoxyphenyl)methyl (+)-4-(difluoromethoxy)-α-(1-methylethyl) benzeneacetate **F43**
 cyano(3-phenoxyphenyl)methyl 2,2-dimethyl-3-(1,2,2,2-tetrabromoethyl)cyclopropanecarboxylate **T194**
 cyano(3-phenoxyphenyl)methyl-2,2,3,3-tetramethylcyclopropanecarboxylate **F18**
 O-(4-cyanophenyl) O,O-dimethyl phosphorothioate **C486**
 cyanophos **C486**
 1-cyanopropane **B289**
 2-cyanopropane **I99**
 2-cyanopropan-2-ol **A18**
 2-cyano-1-propene **M108**
 2-cyanopyridine **C487**
 3-cyanopyridine **C488**
 4-cyanopyridine **C489**
 Cyanosil **H100**
 3-cyanotoluene **T188**
 4-cyanotoluene **T190**
 o-cyanotoluene **T189**
 ω-cyanotoluene **B97**
 cyanotrichloromethane **T229**
 Cyanox **C486**
 Cyanox LTDP **D365**
 cyanthoate **C490**
 cyanuramide **M47**
 cyanurchloride **C492**
 cyanuric acid **C491**
 cyanuric acid chloride **C492**
 cyanuric chloride **C492**
 cyanuric fluoride **C493**
 cyanuric trichloride **C492**
 cyanurotriamide **M47**
 Cybet **C498**
 Cybolt **F43**
 cycasin **C494**
 cyclamate sodium **S59**
 cyclamic acid **C495**
 cyclandelate **C496**
 cyclic methylene-diethoxyphosphinodithiomidocarbonate **F109**
 cyclic N',O-propylene ester of N,N-bis(2-chloroethyl)-phosphorodiamidic acid monohydrate **C529**
 cyclic tetramethylene sulfone **S143**
 cyclizine **C497**
 α-cycloamylose **C500**
 β-cycloamylose **C501**
 cycloate **C498**
 Cyclobet **C498**
 cyclobutane-1,3-dione **C499**
 α-cyclocitrylideneacetone **I57**
 α-cyclodextrin **C500**
 β-cyclodextrin **C501**
 γ-cyclodextrin **C502**
 αcyclodextrin hydrate **C500**
 cyclododecane morpholine derivative **D593**
 (E,E,E)-1,5,9-cyclododecatiene **C503**
 (E,E,Z)-1,5,9-cyclododecatiene **C504**
 trans,trans,cis-1,5,9-cyclododecatiene **C504**
 4-cyclododecyl-2,6-dimethylmorpholine acetate **D593**
 cycloheptaamylose **C501**
 cycloheptane **C505**
 cycloheptatriene **C506**
 1,3,5-cycloheptatriene **C506**
 cyclohexaamylose **C500**
 1,4-cyclohexadienedione **B74**
 2,5-cyclohexadiene-1,4-dione **B74**
 3,5-cyclohexadiene-1,2-dione **B73**
 2,5-cyclohexadiene-1,4-dione dioxime **B75**
 cyclohexamethylenimine **H56**
 cyclohexanamine **C514**
 cyclohexane **C507**
 cyclohexanecarbamic acid, N-ethylthio-, S-ethyl ester **C498**
 cyclohexane-4-carboxaldehyde **T71**
 cyclohexanecarboxylic acid, 2,2-dimethyl-4,6-dioxo-5-[1-[(2-propenyloxy)imino]butyl]-, methyl ester, ion(1-), sodium **A71**
 trans-1,2-cyclohexanedicarboxylic acid **H49**
 cis-1,2-cyclohexanedicarboxylic anhydride **H50**
 cyclohexane, 2,4-diisopropenyl-1-methyl-1-vinyl-, (1α,2β,4β)- **E14**
 cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1α,2β,4β)]- **E14**
 cis-1,2,3,5-trans-4,6-cyclohexanehexol **I37**
 1,2,3,4,5,6-cyclohexanehexolphosphoric acid **P180**
 cyclohexanehexyl hexaphosphate **P180**
 cyclohexanesulfamic acid **C495**
 cyclohexanethiol **C518**
 cyclohexanol **C508**
 cyclohexanol, 1-[(1-hydroperoxycyclohexyl)dioxy]- **C510**
 cyclohexanone **C509**
 cyclohexanone hydroperoxide **C510**
 cyclohexene **C511**
 3-cyclohexene-1-carboxaldehyde **T71**
 4-cyclohexene-1,2-dicarboximide, N-[trichloromethyl]thio]- **C59**
 cyclohex-4-ene-1,2-dicarboxylic anhydride **T76**
 2-cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)-, (S)- **C93**
 5-(1-cyclohexen-1-yl)-1,5-dimethylbarbituric acid **H76**
 5-(1-cyclohexen-1-yl)-1,5-dimethyl-2,4,6 (1H,3H,5H)-pyrimidinetrione **H76**
 cyclohexenylethylene **V31**
 3-cyclohexenyltrichlorosilane **C512**
 cycloheximide **C513**
 3-cyclohexyl-1-(p-acetylphenylsulfonyl)urea **A15**
 cyclohexyl alcohol **C508**
 cyclohexylamine **C514**
 cyclohexylamine sulfate **C515**
 N-cyclohexylcyclohexanamine **D265**
 N-cyclohexylcyclohexanamine nitrite **D266**
 cyclohexyldimethylamine **D411**
 N-cyclohexyldimethylamine **D411**
 3-cyclohexyl-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4(1H,3H)-dione **H69**

3-cyclohexyl-6-(dimethylamino)-1-methyl-s-triazine-2,4(1*H*,3*H*)-dione **H69**
 2-cyclohexyl-4,6-dinitrophenol **C516**
 1-cyclohexyldodecane **D590**
 cyclohexyl isocyanate **C517**
 cyclohexyl mercaptan **C518**
 cyclohexylmethane **M197**
N-cyclohexyl-*N*-methoxy-2,5-dimethyl-3-furancarboxamide **F130**
 cyclohexylsulfamic acid **C495**
 Cyclomycin **T62**
 Cyclon **H86**
 Cyclon **H100**
 Cyclone **P11**
 Cyclone B **H100**
 cyclonite **R2**
 cyclooctaamylose **C502**
 1,5-cyclooctadiene **C519**
cis,cis-1,5-cyclooctadiene **C520**
(Z,Z)-1,5-cyclooctadiene **C520**
 cyclooctapentylolose **C502**
 cyclooctatetraene **C521**
 3-cyclooctyl-1,1-dimethylurea **C532**
 cyclooxabutane **T309**
 Cyclopan **H76**
 cyclopentadiene **C528**
 cyclopenta-1,3-diene **C528**
 1,3-cyclopentadiene, dimer **D271**
 cyclopentadienylmanganese tricarbonyl **M23**
 cyclopenta[*de*]naphthalene **A4**
 cyclopentane **C522**
 cyclopentane-1,2,3,4-tetracarboxylic acid **C523**
 cyclopentanol **C524**
 cyclopentanone **C525**
 4*H*-cyclopenta[*def*]phenanthrene **C526**
 1*H*-cyclopentapyrimidine-2,4(3*H*,5*H*)-dione, 3-cyclohexyl-6,7-dihydro- **L34**
 cyclopentene **C527**
 cyclopentene epoxide **O43**
 cyclopentene oxide **O43**
 2-cyclopenten-1-one, 2-allyl-4-hydroxy-3-methyl-2,2-dimethyl-3-(2-methylpropenyl)cyclopropanecarboxylate **A68**
 1,3-cyclopentadiene **C528**
 cyclopentimine **P201**
 cyclopentylalcohol **C524**
 2-cyclopentyl-4-chlorophenol **C189**
 cyclophosphamide **C529**
 cyclophosphan **C529**
 cyclophosphoramidate **C529**
 cyclopropane **C530**
 cyclopropanecarboxamide, *N*-(3-chlorophenyl)-*N*-(tetrahydro-2-oxo-3-furanyl)- **C544**
 cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester **C542**
 cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, (3-phenoxyphenyl)methyl ester **P56**
 cyclopropanecarboxylic acid, 3-[(dihydro-2-oxo-3(2*H*)-thienylidene)methyl]-2,2-dimethyl-, [5-(phenylmethyl)-3-furanyl]methyl ester, [1*R*-[1*α*,3*α*(*E*)]- **K1**
 cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, [5-(phenyl methyl)-3-furanyl]methyl ester **R4**
 cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, (5-benzyl-3-furyl)methyl ester **R4**
 cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2-pentenyl)-2-cyclopenten-1-yl ester, [1*R*-[1*α*[*S**(*Z*),3*β*(*E*)]- **J1**
 cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2-propenyl)-2-cyclopenten-1-yl ester **A68**
 cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, *m*-phenoxybenzyl ester **P84**
 cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, (3-phenoxyphenyl)methyl ester **P84**
 α -cyclopropyl- α -14-methoxyphenyl-5-pyrimidinemethanol **A207**
N-(cyclopropylmethyl)- α,α,α -trifluoro-2,6-dinitro-*N*-propyl-*p*-toluidine **P281**
 Cyclor **C498**
 Cyclosan **M70**
 cyclosporin A **C531**
 Cycloten **M31**
 Cyclotene **M31**
 cyclotrimethylenenitramine **R2**
 cycluron **C532**
 Cycogan **C141**
 cyclolamin **C368**
 cyfluthrin **C533**
 Cygon **D376**
 cyhalothrin **C534**
 cyhexatin **C535**
 Cymag **S58**
 Cymantrene **M23**
 cymarin **C536**
 cymene **C537**
m-cymene **C538**
o-cymene **C539**
p-cymene **C540**
 cymol **C537**
 cymoxanil **C541**
 Cynkotox **Z9**
 Cynock **C486**
 Cynophos **T135**
 Cyodrin **M167**
 Cyofrem **C141**
 Cyolane **P151**
 Cyomin **C368**
 cypentil **P201**
 cypermethrin **C542**
 α -cypermethrin **C543**
 Cypha **C534**
 cyprofuram **C544**
 Cypromate **P307**

Cyren **S116**
 cyromazine **C545**
 Cystospaz **H124**
 cytarabine **C546**
 cytembena **C547**
 Cythrin **F43**
 Cytosar-U **C546**
 1-(1'-cytosinyl)-4-[L-3'-amino-5'-(1''-N-methylguanidino)-valerylamino]-1,2,3,4-tetra-deoxy- β -*erythro*-hex-2-enuronic acid **B139**
 cytoal alcohol cyclohexylammonium salt **C548**
 Cytosan **C529**
 cytrol **A160**
 Cytrolane **M56**
 D-50 **P348**
 1,3-D **D250**
 2,4-D **D1**
 2,4-D, amine salt **D2**
 2,4-D, ammonium salt **D2**
 2,4-D-butotyl **D3**
 2,4-D, butoxyethanol ester **D3**
 2,4-D, butyl ester **D4**
 2,4-D, *sec*-butyl ester **D5**
 2,4-D, 4-chloro-2-butenyl ester **D6**
 2,4-D, diethylamine salt **D7**
 2,4-D, diethylammonium salt **D7**
 2,4-D, dimethylammonium salt **D8**
 2,4-D, lithium salt **D12**
 2,4-D, isopropyl ester **D11**
 2,4-D, methyl ester **D13**
 2,4-D,2-methylpropyl ester **D9**
 2,4-D, octyl ester **D14**
 2,4-D, propylene glycol butyl ether ester **D15**
 2,4-D, sodium salt **D16**
 3,4-D **D239**
 D70 **H37**
 DZ **P120**
 3,4-DA **D239**
 DAA **D65**
 2,4-DAA **D73**
p-DAB **D387**
 Dabinese **C311**
 Dacamine **T1**
 Dacamox **T131**
 dacarbazine **D17**
 Daconate **M355**
 Daconil **C286**
 DACPM **M210**
 Dacthal **C317**
 Dactinomycin **A46**
 DADI **D379**
 DADPS **S146**
 Dagger **I5**
 daidzein **D18**
 daidzeol **D18**
 Daiflon S3 **T269**
 Daimichi yellow G **D96**
 daimuron **D603**
 Daiwa Brilliant Blue FCF **C387**
 Daiwa Carmoisine **C393**
 Daiwa Orange G **C392**
 Daiwa Patent Blue VX **C386**
 Daiwa Ponceau R **C395**
 Daiwa Uranine **C399**
 dalapon **D19**
 dalapon-sodium **D20**
 dambose **I37**
 Damfin **M102**
 daminozide **D21**
 Danantizal **M122**
 Danitol **F18**
 Danitron **F21**
 danthron **D22**
 Dantoin **D205**
 dantoin DMDMH 55 **D446**
 dantron **D22**
 DAP **D72**
 Dapon 35 **D72**
 Dapsone **S146**
 Daraprim **P361**
 Darlem **P145**
 Darvon **P319**
 Darvon N **P320**
 Dash **G18**
 Dasonit **F23**
 2,4-DAT **D87**
 2,6-DAT **D90**
 Daturine **H124**
 daunomycin **D23**
 daunorubicin **D23**
 Davron **P318**
 dazomet **D24**
 2,4-DB **D25**
 DBA **D589**
 DBA **D103**
 DB[*a,h*]A **D103**
 DB[*a,j*]AC **D102**
 DBCM **D126**
 DBCP **D128**
 DBED **B45**
 2,4-D(BEE) **D3**
 DBHMD **D146**
 DBN **D166**
 DBNA **N146**
 DBNPA **D135**
 DBNPG **D134**
 DBP **D160**
 DBP **D137**
 DB[*a,e*]P **D115**
 DB[*a,h*]P **D116**
 DB[*a,i*]P **D117**
 DBPC **B245**
 DBPP **D159**
 DC 360 **S32**

DCA **D182**
DCA **D172**
D & C Acid Red No. 87 **E29**
DCB **D188**
DCB **D200**
DCC **D267**
DCCD **D267**
DCCI **D267**
DCDD **D105**
DCIP **D26**
DCMU **D579**
DCNU **C307**
DCP **D237**
3,4-D CPA **P295**
DCPC **C125**
DCPE **C125**
D & C Red 9 **D27**
D & C Red No.15 **C414**
D & C Red No. 22 **E29**
D & C Red No. 35 **C416**
D & C Yellow 11 **C427**
D & C Yellow No. 10 **Q10**
D-D **D28**
D&D **Q1**
DDC **S64**
DDD **D30**
o,p'-DDD **D29**
p,p'-DDD **D30**
DDDM **D235**
p,p'-DDD olefin **D33**
DDE **D31**
4,4'-DDE **D31**
p,p'-DDE **D31**
ddI **D273**
ddIno **D273**
DDM **M218**
p,p'-DDMS **D32**
p,p'-DDMU **D33**
cis-DDP **C350**
DDS **S146**
DDT **D35**
4,4'-DDT **D35**
o,p'-DDT **D34**
p,p'-DDT **D35**
DDVP **D258**
DDX 6202 **Q13**
2,4-DE **D7**
DEA **D288**
Deadline **B152**
DEAE **D289**
Debantic **T60**
debrisoquine **D36**
decaborane **D37**
decaborane(14) **D37**
nido-decaborane(14) **D37**
decaboron tetrahydride **D37**
decabromodiphenyl ether **P24**
decabromodiphenyl oxide **P24**
decachlor **D277**
1,1',2,2',3,3',4,4',5,5'-decachlorobis(2,4-cyclopentadien-1-yl) **D277**
decachlorobis(2,4-cyclopentadien-1-yl) **D277**
1,1*a*,3,3*a*,4,5,5*a*,5*b*,6-decachlorooctahydro-1,3,4-metheno-2*H*-cyclobuta[*cd*]pentalen-2-one **C119**
decachlorotetrahydro-4,7-methanoindeneone **C119**
Decaderm **D62**
cis-decahydronaphthalene **D38**
trans-decahydronaphthalene **D39**
cis-decalin **D38**
trans-decalin **D39**
decamethrin **D46**
decamethylene dibromide **D129**
decanal **D40**
1-decanal **D40**
decane **D41**
n-decane **D41**
1-decanecarboxylic acid **U4**
decanedioic acid **S11**
1-decanol **D42**
Decap **D458**
Decapryn succinate **D599**
decarbofuran **D43**
Deccosil **I4**
Deccotane **B240**
Decemthion **P153**
dechlorane **M334**
declomycin **D47**
declomycin hydrochloride **D48**
Decorpa **G51**
decyl alcohol **D42**
n-decyl alcohol **D42**
decyl aldehyde **D40**
1-decylaldehyde **U1**
decylbenzene **D44**
n-decylbenzene **D44**
N-decyl-*N,N*-dimethyl-1-decanaminium chloride **D274**
n-decyl *n*-octyl phthalate **O22**
decyl phthalate **D275**
Dedevap **D258**
Ded-weed **T1**
Deenax **B245**
deep lemon yellow **S122**
DEET **D319**
o-DEET **D320**
p-DEET **D321**
DEF **E68**
Defanet **D374**
DEF defoliant **T209**
Deflexol **Z25**
Defoal **M3**
DEG **D301**
Degamin IPDA **I111**
Degranol **M29**
DE-Green **T209**

DEH 26 **T65**
 Dehistin **T334**
 DEHP **D519**
 dehydrite **M7**
 dehydroacetic acid **D45**
 dehydroacetic acid, sodium salt **S60**
 7-dehydrocholesterol, activated **C323**
 1-dehydrocortisone **P269**
 dehydrogen monosulfide **H105**
 6-dehydro-6-methyl-17 α -acetoxypregesterone **M44**
 dehydrothio-*p*-toluidine **A145**
 Dehyquart C **L10**
 Delac J **N155**
 Delaflo **C44**
 Delaglas-A **P226**
 Delan **D570**
 Delaprism **P226**
 Deleaf defoliant **M89**
 Delnav **D531**
 Delowax S **T28**
 Delowax OM **T28**
 Delpet **P226**
 delphinic acid **I141**
 Delros **B137**
 delsterol **C323**
 Delta **C238**
 Deltacortil **P269**
 Deltalin **E42**
cis-deltamethin **D46**
 deltamethrin **D46**
 deltamethrine **D46**
 Deltanet **F125**
 Delu Wuehlmaus-Gas **C24**
 Demand **C534**
 demeclocycline **D47**
 demeclocycline hydrochloride **D48**
 Demeon D **D413**
 demethylchlortetracycline **D47**
 demethylfenitrothion **P14**
 demeton **D49**
 demeton-methyl **D50**
 demeton-*O*-methyl **D52**
 demeton-*S*-methyl **D54**
 demeton-*S*-methylsulfon **D55**
 demeton-*S*-methyl sulfone **D55**
 demeton-*O* **D51**
 demeton-*S* **D53**
 demeton-*S* sulfone **D56**
 demeton sulfone **D56**
 demeton thiol sulfone **D56**
 demetonthione **D51**
 De-Mice **B150**
 Demise **F11**
 Demitan **F6**
 DEN **N149**
 DENA **N149**
 Dendrid **I48**
 2-deoxy-4-*O*-(2,6-diamino-2,6-dideoxy- α -D-glucopyranosyl)-D-streptamine **N35**
 6-deoxy-D-galactose **F114**
 2'-deoxy-5-iodouridine **I48**
 (S)-7-[[6-*O*-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy] hesperetin **H30**
 3-[(6-deoxy- α -L-mannopyranosyl)oxy]-1,5,11 α ,14,19-pentahydroxycard-20(22)-enolide **O40**
 2-deoxy-2-[[[(methylnitrosoamino)carbonyl]amino]-D-glucose **S120**
 3-deoxynorlutin **L67**
 1-(2-deoxy- β -D-ribofuranosyl)-5-iodouracil **I48**
 Deoxy-Sol **H87**
 deoxyteraric acid **M15**
 DEP **T225**
 DEP **D314**
 Depakine **V8**
 Deparal **C323**
 Depocid **S139**
 Deprinol **I15**
 Dequest 2010 **E183**
 Dequest 2040 **E11**
 Deracil **T145**
 Derfon **D315**
 Deriton **M349**
 Dermacourt **H95**
 Dermadex **H41**
 Dermafos **F8**
 Dermistine **D537**
 Dermoxyl **B83**
 Derris **R18**
 DES **S116**
 deschlorobiomycin **T62**
 deserpidine **D58**
 deserpine **D58**
 Desical **C37**
 desmedipham **D59**
 Desmel **P306**
 11-desmethoxyreserpine **D58**
 des-*N*_a-methyl-*N*_a-formylvinblastine sulfate **V25**
 desmetryn **D60**
 Desmetryne **D60**
 Desoxon 1 **P51**
 2-desoxyphenobarbital **P272**
 Despirol **K6**
 2,4-DES-sodium **D57**
 Destun **P54**
 DETA **D319**
o-DETA **D320**
p-DETA **D321**
 Detectas Orange 201 **C426**
 Detergent Alkylate No.2 **P100**
 Dethmor **W1**
 DETP **T225**
 detricine **D17**
 deuterium **D61**
 Devarcid Fast Orange 2GS **C392**

Devarcid Orange II **C391**
 Devarcid Uranine SSO **C399**
 Devar Ponceau R **C395**
 Developer Z **P121**
 Developer H **P101**
 Developer PF **P103**
 Dever Brilliant Blue FCF **C411**
 Devicorun **I137**
 Devrinol **N28**
 6-F-DEW **N145**
 Dextracont **D62**
 dexamethasone **D62**
 Dexason **D62**
 Dexon **F2**
 dextromethorphan **D63**
 dextromethorphan hydrobromide **D64**
 dextropropoxyphene **P318**
 dextropropoxyphene hydrochloride **P319**
 dextropropoxyphene napsylate **P320**
 dextrose **G17**
 dextrowarfarin **W2**
 dezodorator **N9**
 DFT **T123**
 DGBA **B228**
 DHA **D45**
 DHPT **A145**
 DHT 4A **H108**
 Diabefagos **M100**
 Diabetol **T171**
 Diabinese **C311**
 Diacel Navy DC **D95**
 4,4'-diacetamidobiphenyl **D67**
 diacetic ether **E88**
 diacetone **D65**
 diacetone alcohol **D65**
 3 β ,17 β -diacetoxy-17 α -ethynyl-4-estrene **E182**
 3 β ,17 β -diacetoxy-17 α -ethynyl-4-oestrene **E182**
 diacetoxymercury **M65**
 diacetyl **B209**
 diacetylbenzidine **D67**
 4,4'-diacetylbenzidine **D67**
 1,2-diacetylene **H62**
 α,β -diacetylene **H62**
 diacetylmethane **A22**
 diacetyl peroxide **D66**
 Diafuran **C68**
 Dialifor **D68**
 dialifos **D68**
 diallate **D69**
 di-allate **D69**
 diallylamine **D70**
N,N-diallylchloroacetamide **A69**
N,N-diallyldichloroacetamide **D171**
N,N-diallyl-2,2-dichloroacetamide **D171**
 diallyl ether **D71**
 diallyl phthalate **D72**
 diallyl *o*-phthalate **D72**
 Diamal **M11**
 Diameaat **T134**
 diamide **H87**
 Diamine H Extra **H54**
 3,6-diaminoacridinium chloride **P280**
 3,6-diaminoacridinium hydrochloride **P280**
 2,4-diaminoanisole **D73**
 2,4-diaminoanisole sulfate **D74**
 1,2-diamino-9,10-anthracenedione **D75**
 1,4-diamino-9,10-anthracenedione **D76**
 1,5-diamino-9,10-anthracenedione **D77**
 2,6-diamino-9,10-anthracenedione **D78**
 1,2-diaminoanthraquinone **D75**
 1,4-diaminoanthraquinone **D76**
 1,5-diaminoanthraquinone **D77**
 2,6-diaminoanthraquinone **D78**
 2,4-diaminoazobenzene **D79**
 2,4-diaminoazobenzene hydrochloride **C341**
 1,2-diaminobenzene **P102**
m-diaminobenzene **P101**
p-diaminobenzene **P103**
 1,3-diaminobenzene dihydrochloride **P104**
 4,4'-diaminobiphenyl **B52**
 1,3-diaminobutane **B200**
 1,4-diaminobutane **B201**
 1,2-diamino-4-chlorobenzene **C245**
 3,4-diamino-1-chlorobenzene **C245**
 2,4-diamino-5-(*p*-chlorophenyl)-6-ethylpyrimidine **P361**
N,N'-(2,5-diamino-2,5-cyclohexadiene-1,4-diylidene)bis-1,4-benzenediamine **B2**
 4,4'-diamino-3,3'-dichlorobiphenyl **D192**
 4,4'-diaminodicyclohexylmethane **D272**
O-(2,6-diamino-2,6-dideoxy- α -D-glucopyranosyl-(1 \rightarrow 4)-*O*-[2,6-diamino-2,6-dideoxy- β -L-idopyranosyl-(1 \rightarrow 3)- β -D-ribofuranosyl]-(1 \rightarrow 5)]-2-deoxy-D-streptami **N36**
 2,2'-diaminodiethylamine **D303**
 2,4'-diaminodiphenyl **D543**
 diaminodiphenyl ether **O58**
 4,4'-diaminodiphenyl ether **O58**
 2,4'-diaminodiphenylmethane **M217**
 4,4'-diaminodiphenylmethane **M218**
o,p'-diaminodiphenylmethane **M217**
p,p'-diaminodiphenylmethane **M218**
p,p'-diaminodiphenyl sulfide **T127**
 4,4'-diamino diphenyl sulfone **S146**
 3,3-diaminodipropylamine **N208**
 1,2-diaminoethane **E114**
 1,2-diaminoethane copper complex **C477**
 2,7-diamino-10-ethyl-9-phenylphenanthridinium bromide **E65**
 3,8-diamino-5-ethyl-6-phenylphenanthridinium bromide **E65**
 1,6-diaminohexane **H54**
 1,2-diamino-3-methylbenzene **D86**
 1,2-diamino-4-methylbenzene **D92**
 1,3-diamino-2-methylbenzene **D90**
 1,3-diamino-4-methylbenzene **D87**

2,4-diamino-1-methylbenzene **D87**
 1,5-diaminonaphthalene **N10**
 1,2-diamino-4-nitrobenzene **N134**
 1,4-diamino-2-nitrobenzene **N133**
 2,4-diamino-6-(5-nitro-2-furyl)-s-triazine **D80**
 2,4-diaminophenol **D81**
 2,4-diaminophenol dihydrochloride **D82**
 diaminophenol hydrochloride **D82**
 2,6-diamino-3-(phenylazo)-pyridine **P62**
p,p'-diaminophenyl ether **O58**
 3,7-diamino-5-phenylphenazinium chloride **P82**
 di(*p*-aminophenyl) sulfide **T127**
 1,2-diaminopropane **D83**
 1,3-diaminopropane **D84**
 di(3-aminopropyl)amine **N208**
 (((diaminopteridiny)methyl)amino)benzoylglutamic acid **A150**
N-(4-[(2,4-diamino-6-pteridiny)methyl]methyl-amino)benzoyl-L-glutamic acid **M128**
N-(*p*-(2,4-diamino-6-pteridylmethyl)amino)benzoylglutamic acid **A150**
 diaminostilbenedisulfonic acid **D85**
 4,4'-diamino-2,2'-stilbenedisulfonic acid **D85**
 2,3-diaminotoluene **D86**
 2,4-diaminotoluene **D87**
 2,5-diaminotoluene **D88**
 2,6-diaminotoluene **D90**
 3,4-diaminotoluene **D92**
 3,5-diaminotoluene **D93**
 2,6-diaminotoluene dihydrochloride **D91**
 2,5-diaminotoluene sulfate **D89**
 5-[(4,6-diamino-1,3,5-triazin-2-yl)methyl] *O,O*-dimethyl phosphorodithioate **M50**
 2,4-diamino-5-(3,4,5-trimethoxybenzyl)pyrimidine **T302**
 1,3-diaminourea **C69**
 diammonium fluosilicate **A174**
 diammonium hexafluorosilicate **A174**
 diammonium monohydrogen arsenate **A163**
 diammonium oxalate **D94**
 diammonium peroxodisulfate **A181**
 diammonium sulfate **A185**
 diammonium sulfide **A186**
 diammonium trisulfide **A183**
 diamylamine **D533**
 di-*n*-amylamine **D533**
 diamyl ether **P48**
 diamyl ketone **U7**
 diamyl phthalate **D534**
 1,2,3,4-dianhydroerythritol **D280**
 1,4:3,6-dianhydro-*D*-glucitol **I137**
 1,2:3,4-dianhydrothriitol **D279**
o,p'-dianiline **D543**
o-dianisidine **D95**
 dianisidine diisocyanate **D379**
 diantimony trioxide **A227**
 diarsenic trioxide **A244**
 diarsenic trisulfide **A245**
 diarthon **D22**
 Diarylanilide Yellow **D96**
 Diastatin **N210**
 diatol **D298**
 diatomaceous earth **D97**
 diatomite **D97**
 Diawa Acid Rhodamine B **C396**
 9,10-diazaanthracene **P61**
 1,9-diazafluorene **C70**
 2,9-diazafluorene **C71**
 9*H*-1,9-diazafluorene **C70**
 1,2-diazaindene **I22**
 1,3-diazaindene **B53**
 Diazald **M269**
 Diazale **M269**
 3,6-diazaoctane-1,8-diamine **T284**
 4,5-diazaaphenanthrene **P60**
 diazenedicarboxamide **A271**
 diazene, diphenyl 1-oxide **A274**
 diazepam **D98**
 diazinon **D99**
 diazirine **D100**
 diazoacetate (ester)-1-serine **A260**
O-diazoacetyl-1-serine **A260**
 Diazoben **M271**
 diazobenzene **A268**
 Diazo Fast Red B **M141**
 diazoimide **H97**
 2-diazoindan-1,3-dione **P175**
 1,2-diazole **P349**
 1,3-diazole **I9**
 diazomethane **D100**
 Diazyl **S132**
 DIBA **D351**
 Dibar **F27**
 dibarium trisulfide **B22**
 dibasic lead phosphite **L28**
 dibasic sodium phosphate **S79**
 dibasic zinc stearate **Z16**
 1,2,5,6-dibenzacridine **D101**
 1,2,7,8-dibenzacridine **D102**
 3,4,5,6-dibenzacridine **D102**
 dibenz[*a,d*]acridine **D101**
 dibenz[*a,f*]acridine **D102**
 dibenz[*a,h*]acridine **D101**
 dibenz[*a,j*]acridine **D102**
 1,2,5,6-dibenzanthracene **D103**
 1,2,5,6-dibenz[*a*]anthracene **D103**
 1,2,7,8-dibenzanthracene **D103**
 dibenz[*a,h*]anthracene **D103**
 dibenz[*de,kl*]anthracene **P57**
 5*H*-dibenz[*b,f*]azepine-5-carboxamide **C61**
 1,2,5,6-dibenzoacridine **D101**
 1,2,5,6-dibenzoanthracene **D103**
 dibenzo[*a,h*]anthracene **D103**
 3,4,5,6-dibenzocarbazole **D104**
 7*H*-dibenzo[*c,g*]carbazole **D104**

dibenzo[*b,def*]chrysene **D116**
dibenzo[*def,mno*]chrysene **D119**
dibenzo[*b,def*]chrysene-7,14-dione **C428**
dibenzo-*p*-dioxin **D106**
dibenzo[1,4]dioxin **D106**
dibenzo[*b,e*][1,4]dioxin **D106**
dibenzo-*p*-dioxin, 1-chloro- **D107**
dibenzo-*p*-dioxin, 2-chloro- **D108**
dibenzo-*p*-dioxin, 1,6-dichloro- **D109**
dibenzo-*p*-dioxin, 2,7-dichloro- **D105**
dibenzo-*p*-dioxin, 1,2,3,7,8,9-hexachloro- **H37**
dibenzo-*p*-dioxin, 2,3,7,8-tetrachloro- **D110**
dibenzo[*a,j,k*]fluorene **B58**
dibenzo[*b,j,k*]fluorene **B59**
dibenzofuran **D111**
dibenzo[*b,d*]furan **D111**
3-dibenzofuranamine **D114**
dibenzofuran, chlorinated **D112**
dibenzofuran, polychlorinated **D113**
1,2,5,6-dibenzonaphthalene **C340**
dibenzoparadiazine **P61**
dibenzo PQD **B75**
dibenzopyrazine **P61**
1,2,3,4-dibenzopyrene **D118**
1,2,6,7-dibenzopyrene **D116**
1,2,9,10-dibenzopyrene **D118**
1,2,4,5-dibenzopyrene **D115**
1,2,7,8-dibenzopyrene **D117**
2,3,4,5-dibenzopyrene **D118**
3,4,8,9-dibenzopyrene **D116**
3,4,9,10-dibenzopyrene **D117**
4,5,6,7-dibenzopyrene **D118**
dibenzo[*a,e*]pyrene **D115**
dibenzo[*a,h*]pyrene **D116**
dibenzo[*a,i*]pyrene **D117**
dibenzo[*a,l*]pyrene **D118**
dibenzo[*b,h*]pyrene **D117**
dibenzo[*cd,jh*]pyrene **D119**
dibenzo[*cd,jk*]pyrene **D119**
2,3,5,6-dibenzopyridine **A34**
dibenzo(*b,e*)pyridine **A34**
dibenzo- γ -pyrone **X3**
dibenzopyrrole **C64**
dibenzothiazine **P83**
dibenzothiazyl disulfide **D572**
dibenzoyl peroxide **B83**
1',2',6',7'-dibenzpyrene-7,14-quinone **C428**
dibenzyl ether **D120**
N,N'-dibenzylethylenediamine **B45**
dibenzylene chloride **P85**
dibenzylene hydrochloride **P85**
dibismuth tritelluride **B132**
DIBK **D353**
Di-Blox **D535**
diborane **D121**
diborane(6) **D121**
diboron hexahydride **D121**
diboron trioxide **B144**
Dibrom **N3**
dibromoacetonitrile **D122**
2,4-dibromo-1-anthraquinololylamine **A125**
4,4'-dibromobenzelic acid isopropyl ester **B187**
dibromobenzene **D123**
1,4-dibromobenzene **D124**
p-dibromobenzene **D124**
4,4'-dibromobenzilate **B187**
4,4'-dibromobiphenyl **D125**
4,4'-dibromo-1,1'-biphenyl **D125**
p,p'-dibromobiphenyl **D125**
1,3-dibromo-2,2-bis(bromomethyl)propane **P37**
3,5-dibromo-*N*-(4-bromophenyl)-2-hydroxybenzamide **T208**
dibromochloromethane **D126**
2,6-dibromo-4-chlorophenol **D127**
dibromochloropropane **D128**
1,2-dibromo-3-chloropropane **D128**
dibromocyanoacetamide **D135**
2,2-dibromo-2-cyanoacetamide **D135**
 α,α -dibromo- α -cyanoacetamide **D135**
2,6-dibromo-4-cyanophenol **B189**
1,10-dibromodecane **D129**
dibromodichloromethane **D130**
1,2-dibromo-2,4-dicyanobutane **B163**
dibromodifluoromethane **D131**
4,4'-dibromodiphenyl ether **B115**
1,2-dibromoethane **D132**
 α,β -dibromoethane **D132**
sym-dibromoethane **D132**
3,5-dibromo-4-hydroxybenzonitrile **B189**
3,5-dibromo-4-hydroxyphenyl cyanide **B189**
3,5-dibromo-2-hydroxy-*N*-[3-(trifluoromethyl)phenyl]benzamide **F72**
dibromomethane **D133**
dibromoneopentyl glycol **D134**
2,2-dibromo-3-nitrilopropionamide **D135**
dibromopentaerythritol **D134**
1,5-dibromopentane **D136**
di-4-bromophenyl ether **B115**
2,3-dibromopropanal **A38**
2,3-dibromopropanol **D137**
2,3-dibromopropan-1-ol **D137**
2,3-dibromopropionaldehyde **A38**
2,3-dibromopropyl alcohol **D137**
3,5-dibromo- α,α -trifluoro-*m*-salicyl-*o*-toluidide **F72**
Dibromphos **N3**
dibutalin **B232**
1,2-dibutoxyethane **D138**
dibutoxyethoxyethyl adipate **D139**
dibutyl acid phosphate **D147**
dibutyl adipate **D140**
di-*n*-butyl adipate **D140**
dibutylamine **D141**
di-2-butylamine **D142**
di-*sec*-butylamine **D142**

N-dibutylamine **D141**
 dibutylaminoethanol **D143**
 2-(dibutylamino)ethanol **D143**
 2-dibutylaminoethanol **D143**
 2-di-*n*-butylaminoethanol **D143**
 2-(*NN*-dibutylamino)ethanol **D143**
N,N-dibutylaminoethanol **D143**
 2,6-di-*tert*-butyl-1,4-benzoquinone **D144**
 2,6-di-*tert*-butyl-*p*-benzoquinone **D144**
 dibutylbis(lauroyloxy)stannane **D163**
 dibutylbis(lauroyloxy)tin **D163**
 dibutylbis[(1-oxododecyl)oxy]stannane **D163**
N,N-dibutyl-1-butanamine **T210**
 dibutyl[1-(butylamino)cyclohexyl]phosphonate **B192**
 dibutyl cellosolve **D138**
 dibutylcellusolve phthalate **B116**
 2,6-di-*tert*-butyl-2,5-cyclohexadiene-1,4-dione **D144**
 dibutylchlorostannane **D161**
 di-*tert*-butylchlorostannane **D162**
 dibutylchlorotin **D161**
 di-*tert*-butylchlorotin **D162**
N,N-dibutylethanolamine **D143**
 dibutyl ether **D145**
S,S-di-*sec*-butyl *O*-ethyl phosphorodithioate **C15**
 dibutylhexamethylenediamine **D146**
N,N'-dibutylhexamethylenediamine **D146**
N,N'-dibutyl-1,6-hexanediamine **D146**
 dibutyl hexanoate **D140**
 dibutyl hydrogen phosphate **D147**
 2,4-di-*tert*-butylhydroxybenzene **D155**
 3,5-di-*tert*-butyl-4-hydroxybenzoic acid **D148**
 dibutylnitrosamine **N146**
 1,3-dibutyl-1-nitrosourea **D149**
N,N'-dibutyl-*N*-nitrosourea **D149**
 dibutyl oxide **D145**
 dibutyl oxitol **D138**
 dibutyloxostannane **D164**
 dibutyloxotin **D164**
 di-*tert*-butyl peroxide **D150**
 2,2-di(*tert*-butylperoxy)butane **D151**
 dibutyl peroxydicarbonate **D152**
 di-*sec*-butyl peroxydicarbonate **D153**
 1,4-di(*tert*-butylperoxyisopropyl)benzene **D154**
 2,4-di-*tert*-butylphenol **D155**
 2,6-di-*tert*-butylphenol **D156**
 3,5-di-*tert*-butylphenol **D157**
N,N'-di-*sec*-butyl-*p*-phenylenediamine **D158**
 dibutyl phenyl phosphate **D159**
 dibutyl phosphate **D147**
 di-*n*-butyl phosphate **D147**
 dibutyl phthalate **D160**
 di-*n*-butyl phthalate **D160**
 dibutyl *o*-phthalate **D160**
 dibutylstannane oxide **D164**
 dibutylstannylene dilaurate **D163**
 di-*tert*-butyltin chloride **D162**
 dibutyltin dichloride **D161**
 di-*n*-butyltin dichloride **D161**
 di-*tert*-butyltin dichloride **D162**
 dibutyltin didodecanoate **D163**
 dibutyltin dilaurate **D163**
 dibutyltin oxide **D164**
 dicamba **D165**
 Dicarbam **C63**
 dicarbomethoxy zinc **Z3**
 di- μ -carbonylhexacarbonyldicobalt **C371**
o-dicarboxybenzene **P172**
 1,2-dicarboxy-3,6-endoxocyclohexane **E22**
 dicarboxymethane **M17**
 dicarboxymethyl sulfide **T130**
 Dicarzol **F102**
 Dicarzol **F103**
 dichlobenil **D166**
 dichlofenthion **D167**
 dichlofluanid **D168**
 dichlone **D169**
 dichloralantipyrine **D170**
 dichloralphenazone **D170**
 2,2'-dichlorethyl ether **B120**
 dichloricide **D190**
 dichloricide aerosol **P221**
 dichloricide mothproofer **P221**
 dichloride- π -cyclopentadienyltitanium **T168**
 dichlorine **C135**
 dichlormid **D171**
 dichloroacetic acid **D172**
 1,1-dichloroacetone **D173**
 1,3-dichloroacetone **D174**
 α,α -dichloroacetone **D173**
 α,α' -dichloroacetone **D174**
 α,γ -dichloroacetone **D174**
sym-dichloroacetone **D174**
 dichloroacetoneitrile **D175**
 dichloroacetyl chloride **D176**
 2,2-dichloroacetyl chloride **D176**
 α,α -dichloroacetyl chloride **D176**
 dichloroacetylene **D177**
 2,3-dichloroallyl chloride **T265**
 5-2,3-dichloroallyl diisopropyl thiocarbamate **D69**
 2,5-dichloro-3-aminobenzoic acid **C110**
 3',5'-dichloro-4-amino-4-deoxy-*N*₁₀-methylpteroglutamic acid **D223**
 2,3-dichloroaniline **D178**
 2,4-dichloroaniline **D179**
 2,5-dichloroaniline **D180**
 2,6-dichloroaniline **D181**
 3,4-dichloroaniline **D182**
 3,5-dichloroaniline **D183**
 4,5-dichloroaniline **D182**
m,p-dichloroaniline **D182**
o,p-dichloroaniline **D179**
 3,6-dichloro-*o*-anisic acid **D165**
 2,3-dichloroanisole **D184**
 2,6-dichloroanisole **D185**

3,5-dichloroanisole **D186**
 2,6-dichlorobenzaldehyde **D187**
 2,4-dichlorobenzeneamine **D179**
 2,6-dichlorobenzeneamine **D181**
 3,4-dichlorobenzeneamine **D182**
 3,5-dichlorobenzeneamine **D183**
 1,2-dichlorobenzene **D188**
 1,3-dichlorobenzene **D189**
 1,4-dichlorobenzene **D190**
m-dichlorobenzene **D189**
o-dichlorobenzene **D188**
p-dichlorobenzene **D190**
 2,6-dichlorobenzene-carbothioamide **C319**
 2,6-dichlorobenzene-methanol **D198**
 4,4'-dichlorobenzidic acid, ethyl ester **C164**
 2,2'-dichlorobenzidine **D191**
 3,3'-dichlorobenzidine **D192**
o,o'-dichlorobenzidine **D192**
o-dichlorobenzidine **D191**
 3,3'-dichlorobenzidine dihydrochloride **D193**
 2,7-dichlorobenzo[*b,e*][1,4]dioxin **D105**
 2,6-dichlorobenzoic acid **D194**
 3,4-dichlorobenzoic acid **D195**
m-dichlorobenzol **D189**
 2,6-dichlorobenzonitrile **D166**
 3,5-dichlorobenzonitrile **D196**
 2,4-dichlorobenzotrichloride **D197**
 di-(4-chlorobenzoyl) peroxide **C171**
 2,6-dichlorobenzyl alcohol **D198**
 3,4-dichlorobenzylammonium chloride, *N*-alkyldimethyl-**A67**
 2,4-dichlorobenzyltributylphosphonium chloride **C309**
 3,3'-dichloro-[1,1'-biphenyl]-4,4'-diamine **D192**
 3,3'-dichloro-(1,1'-biphenyl)-4,4'-diamine dihydrochloride **D193**
 2,2-[(3,3'-dichloro-[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-*N*-phenylbutanamide] **D96**
 3,3'-Dichlorobiphenyl-4,4'-ylenediamine **D192**
 1,1-dichloro-2,2-bis(*p*-chlorophenyl)ethane **D30**
 1,1-dichloro-2,2-bis(*p*-chlorophenyl)ethylene **D31**
 dichlorobis(η⁵-2,4-cyclopentadien-1-yl)hafnium **H3**
 dichlorobis(η⁵-2,4-cyclopentadien-1-yl)titanium **T168**
 dichlorobis(1,1-dimethylethyl)stannane **D162**
 1,1-dichloro-2,2-bis(4-ethylphenyl)ethane **D199**
 4,4'-dichloro-3,3'-bis(trifluoromethyl)carbanilide **F42**
 dichlorobromomethane **B173**
O-(2,5-dichloro-4-bromophenyl) *O*-methylphenylthiophosphonate **L35**
 1,4-dichlorobutene-2 **D200**
 1,4-dichlorobut-2-ene **D200**
 1,4-dichloro-2-butene **D200**
E-1,4-dichloro-2-butene **D201**
trans-1,4-dichlorobutene **D201**
trans-1,4-dichlorobut-2-ene **D201**
trans-1,4-dichloro-2-butene **D201**
 dichlorochlordene **C118**
 2,4-dichloro-6-(*o*-chloroanilino)-*s*-triazine **A208**
 2,4-dichloro-α-(chloromethylene)benzyl alcohol, diethylphosphate **C128**
 1,1-dichloro-2-(*o*-chlorophenyl)-2-(*p*-chlorophenyl)ethane **D29**
 4,6-dichloro-*N*-(2-chlorophenyl)-1,3,5-triazin-2-amine **A208**
 dichloro(2-chlorovinyl)arsine **L41**
 1,3-dichloro-5-cyanobenzene **D196**
 2,6-dichlorocyanobenzene **D166**
 dichlorocyanuric acid **D202**
 2,2-dichloro-*N,N*-diallylacetamide **D171**
cis-dichlorodiamineplatinum(II) **C350**
 3,3'-dichloro-4,4'-diaminobiphenyl dihydrochloride **D193**
 3,3'-dichloro-4,4'-diaminodiphenyl ether **O54**
 3,3'-dichloro-4,4'-diaminodiphenylmethane **M210**
N-3,5-dichloro-4-[[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-L-glutamic acid **D223**
 1,6-dichlorodibenzodioxin **D109**
 1,6-dichlorodibenzo-*p*-dioxin **D109**
 1,6-dichlorodibenzo[*b,e*][1,4]dioxin **D109**
 2,7-dichlorodibenzodioxin **D105**
 2,7-dichlorodibenzo-*p*-dioxin **D105**
 dichlorodibromomethane **D130**
 dichlorodibutylstannane **D161**
 dichlorodi-*tert*-butylstannane **D162**
 dichlorodibutyltin **D161**
 1,1-dichloro-2,2-dichloroethane **T50**
 dichlorodicyclopentadienyltitanium **T168**
 2,2'-dichlorodiethyl-*N*-methylamine *N*-oxide **M39**
 1,2-dichloro-1,1-difluoroethane **D203**
 2,2-dichloro-1,1-difluoroethyl methyl ether **M138**
 dichlorodifluoromethane **D204**
 2,2-dichloro-1,1-difluoro-1-methoxyethane **M138**
 5,5'-dichloro-2,2'-dihydroxydiphenylmethane **D235**
 2,2'-dichlorodiisopropyl ether **D26**
 1,4-dichloro-2,5-dimethoxybenzene **C219**
 1,1-dichloro-*N*-[(dimethylamino)sulfonyl]-1-fluoro-*N*-(4-methylphenyl)methanesulfenamide **T191**
 1,1-dichloro-*N*-[(dimethylamino)sulfonyl]-1-fluoro-*N*-phenylmethanesulfenamide **D168**
 dichlorodimethyl ether **B123**
 α,α'-dichlorodimethyl ether **B123**
 1,3-dichloro-5,5-dimethylhydantoin **D205**
 2,4-dichloro-3,5-dimethylphenol **D256**
 3,5-dichloro-*N*-(1,1-dimethyl-2-propynyl)-benzamide **P339**
 3,5-dichloro-2,6-dimethyl-4-pyridinol **C363**
 dichlorodimethylsilane **D206**
 dichlorodiocetylstannane **D523**
 dichlorodiocetyl tin **D523**
 2,3-dichloro-1,4-dioxane **D207**
 2,3-dichloro-*p*-dioxane **D207**
trans-2,3-dichlorodioxane **D208**
trans-2,3-dichloro-*p*-dioxane **D208**
 dichlorodioxochromium **C339**
 dichlorodiphenylacetic acid **B125**

p,p'-dichlorodiphenylacetic acid **B125**
p,p'-dichlorodiphenyl-2,2-dichloroethane **D30**
 dichlorodiphenylethanol **C125**
 dichlorodiphenylsilane **D209**
 4,4'-dichlorodiphenyl sulfone **B127**
 dichlorodiphenyltrichloroethane **D35**
 2,2-dichloro-*N,N*-di-2-propenylacetamide **D171**
 1,1-dichloroethane **D210**
 1,2-dichloroethane **D211**
 α,β -dichloroethane **D211**
sym-dichloroethane **D211**
 dichloroethanoic acid **D172**
 dichloroethanoyl chloride **D176**
 1,1-dichloroethene **D212**
cis-1,2-dichloroethene **D213**
(E)-1,2-dichloroethene **D214**
trans-1,2-dichloroethene **D214**
(Z)-1,2-dichloroethene **D213**
 2,2-dichloroethenyl dimethyl phosphate **D258**
 1,6-di(2-chloroethylamino)-1,6-dideoxy-D-mannitol dihydrochloride **M29**
 dichloroethylarsine **E112**
 1,1-dichloroethylene **D212**
asym-dichloroethylene **D212**
cis-1,2-dichloroethylene **D213**
trans-1,2-dichloroethylene **D214**
sym-dichloroethyl ether **B120**
 dichloroethyl formal **B118**
 1,1'-dichloroethylidenebis(4-chlorobenzene) **D31**
 1,1'-(2,2-dichloroethylidene)bis[4-ethylbenzene] **D199**
 di(2-chloroethyl)methylamine **M38**
N,N-di(chloroethyl)methylamine **M38**
 dichloroethyl- β -naphthylamine **C142**
 dichloroethylphenylsilane **D215**
 dichloroethyne **D177**
 dichlorofluoromethane **D216**
N-dichlorofluoromethanesulfonyl-*N',N'*-dimethyl-*N*-phenylsulfamide **D168**
N-dichlorofluoromethylthio-*N,N'*-dimethyl-*N*-phenylsulfamide **D168**
N-[(dichlorofluoromethyl)thio]-*N',N'*-dimethyl-*N*-*p*-tolylsulfamide **T191**
 2-[(dichlorofluoromethyl)thio]-1*H*-isindole-1,3-(2*H*)-dione **D217**
N-(dichlorofluoromethylthio)phthalimide **D217**
 2,3-dichloro-*N*-(4-fluorophenyl)maleimide **F67**
 3,4-dichloro-1-(4-fluorophenyl)-1*H*-pyrrole-2,5-dione **F67**
 2,2-dichlorohydrazobenzene **D218**
 dichlorohydrindomethylsilicon **D225**
 dichlorohydrin **D219**
 1,3-dichlorohydrin **D247**
 α,γ -dichlorohydrin **D247**
 2,2-dichloro-*N*-[2-hydroxy-1-(hydroxymethyl)-2-(4-nitrophenyl)ethyl]acetamide **C114**
 2,2-dichloro-*N*-[α R, β R]- β -hydroxy- α -hydroxymethyl-4-nitrophenylethyl]acetamide **C114**
 dichloriodomethane **D220**
 dichloroisocyanurate **D202**
 dichloroisocyanuric acid **D202**
 1,3-dichloroisopropanol **D247**
 dichloroisopropyl ether **D221**
 dichloromethane **D222**
 3',5'-dichloromethopterin **D223**
 dichloromethotrexate **D223**
 3',5'-dichloromethotrexate **D223**
 1,2-dichloro-3-methoxybenzene **D184**
 1,3-dichloro-2-methoxybenzene **D185**
 1,3-dichloro-5-methoxybenzene **D186**
 3,6-dichloro-2-methoxybenzoic acid **D165**
 2,4-dichloro-1-(3-methoxy-4-nitrophenoxy)benzene **C106**
 2-(di(2-chloromethyl)amino)-1-oxa-3-aza-2-phosphacyclohexane 2-oxide monobutylate **C529**
 (dichloromethyl)benzene **B98**
 1,2-dichloro-4-methylbenzene **D255**
 1,3-dichloro-2-methylbenzene **D254**
 2,4-dichloro-1-methylbenzene **D253**
 3,4-dichloro-1-methylbenzene **D255**
 dichloromethyl cyanide **D175**
 2,2-dichloromethyldiethylamine **M38**
 2,2'-dichloro-*N*-methyldiethylamine **M38**
 2,2'-dichloro-*N*-methyldiethylamine, *N*-oxide **M39**
 2,2'-dichloro-4,4'-methylenedianiline **M210**
 4,4'-dichloro-2,2'-methylenediphenol **D235**
sym-dichloromethyl ether **B123**
 3-[2,4-dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2(*H*)-one **O44**
 dichloromethylmethane **D210**
 dichloromethyl methyl ketone **D173**
 3,3-dichloromethyloxacyclobutane **B124**
 dichloromethylphenylsilane **D224**
 dichloromethylsilane **D225**
O-[2,5-dichloro-4-(methylthio)phenyl] *O,O*-diethyl phosphorothioate **C321**
 4,5-dichloronaphthalene-1,8-dicarboxylic anhydride **D226**
 2,3-dichloro-1,4-naphthalenedione **D169**
 6,7-dichloro-1*H*,3*H*-naphtho[1,8-*cd*]pyran-1,3-dione **D226**
 2,3-dichloro-1,4-naphthoquinone **D169**
 4,5-dichloronaphthalic anhydride **D226**
 2,6-dichloro-4-nitroaniline **D260**
 2,6-dichloro-4-nitrobenzenamine **D260**
 1,2-dichloro-3-nitrobenzene **D227**
 1,2-dichloro-4-nitrobenzene **D230**
 1,3-dichloro-4-nitrobenzene **D228**
 1,3-dichloro-5-nitrobenzene **D231**
 1,4-dichloro-2-nitrobenzene **D229**
 2,3-dichloronitrobenzene **D227**
 2,3-dichloro-1-nitrobenzene **D227**
 2,4-dichloronitrobenzene **D228**
 2,4-dichloro-1-nitrobenzene **D228**
 2,5-dichloronitrobenzene **D229**
 3,4-dichloronitrobenzene **D230**
 3,5-dichloronitrobenzene **D231**
o,m-dichloronitrobenzene **D227**
 dichloronitroethane **D232**

1,1-dichloro-1-nitroethane **D232**
 2,4-dichloro-6-nitrophenol **D233**
 2,4-dichloro-1-(4-nitrophenoxy)benzene **N112**
 2',5-dichloro-4'-nitrosalicylanilide **N52**
 2',5-dichloro-4'-nitrosalicylanilide, ethanolamine salt **C362**
 5,2-dichloro-4-nitrosalicylic anilide, 2-aminoethanol salt **C362**
 dichloropalladium **P2**
 1,5-dichloropentane **D234**
 dichlorophen **D235**
 2,3-dichlorophenol **D236**
 2,4-dichlorophenol **D237**
 2,6-dichlorophenol **D238**
 4,6-dichlorophenol **D237**
 2-(2,4-dichlorophenoxy)acetamide **D2**
 (2,4-dichlorophenoxy)acetic acid **D1**
 2,4-dichlorophenoxyacetic acid **D1**
 3,4-dichlorophenoxyacetic acid **D239**
 (3,4-dichlorophenoxy)acetic acid **D239**
 2,4-dichlorophenoxyacetic acid, amine salt **D2**
 (2,4-dichlorophenoxy)acetic acid, amino salt **D2**
 2,4-dichlorophenoxyacetic acid, butoxyethanol ester **D3**
 (2,4-dichlorophenoxy)acetic acid, butoxyethanol ester **D3**
 (2,4-dichlorophenoxy)acetic acid, 2-butoxyethyl ester **D3**
 (2,4-dichlorophenoxy)acetic acid, butyl ester **D4**
 2,4-dichlorophenoxyacetic acid, butyl ester **D4**
 (2,4-dichlorophenoxy)acetic acid, *sec*-butyl ester **D5**
 2,4-dichlorophenoxyacetic acid, *sec*-butyl ester **D5**
 (2,4-dichlorophenoxy)acetic acid, 4-chloro-2-butenyl ester **D6**
 2,4-dichlorophenoxyacetic acid, 4-chloro-2-butenyl ester **D6**
 (2,4-dichlorophenoxy)acetic acid, diethylamine salt **D7**
 2,4-dichlorophenoxyacetic acid, diethylamine salt **D7**
 (2,4-dichlorophenoxy)acetic acid, dimethylamine salt **D8**
 2,4-dichlorophenoxyacetic acid, dimethylamine salt **D8**
 (2,4-dichlorophenoxy)acetic acid, *N*-ethylethanolamine ester **D7**
 (2,4-dichlorophenoxy)acetic acid, isobutyl ester **D9**
 2,4-dichlorophenoxyacetic acid, isobutyl ester **D9**
 2,4-dichlorophenoxyacetic acid, isooctyl ester **D10**
 (2,4-dichlorophenoxy)acetic acid, isooctyl ester **D10**
 2,4-dichlorophenoxyacetic acid, isopropyl ester **D11**
 (2,4-dichlorophenoxy)acetic acid, isopropyl ester **D11**
 (2,4-dichlorophenoxy)acetic acid, lithium salt **D12**
 2,4-dichlorophenoxyacetic acid, lithium salt **D12**
 (2,4-dichlorophenoxy)acetic acid, methyl ester **D13**
 2,4-dichlorophenoxyacetic acid, methyl ester **D13**
 (2,4-dichlorophenoxy)acetic acid, 1-methylethyl ester **D11**
 2,4-dichlorophenoxyacetic acid, 6-methylheptane ester **D10**
 (2,4-dichlorophenoxy)acetic acid, 2-methylpropyl ester **D9**
 (2,4-dichlorophenoxy)acetic acid, monoester with 1,2-propanediol, butyl ether ester **D15**
 (2,4-dichlorophenoxy)acetic acid, octyl ester **D14**
 2,4-dichlorophenoxyacetic acid, octyl ester **D14**
 (2,4-dichlorophenoxy)acetic acid, propylene glycol butyl ether ester **D15**
 2,4-dichlorophenoxyacetic acid, propylene glycol butyl ether ester **D15**
 2,4-dichlorophenoxyacetic acid, sodium salt **D16**
 (2,4-dichlorophenoxy)acetic acid, sodium salt **D16**
 4-(2,4-dichlorophenoxy)butanoic acid **D25**
 2,4-dichlorophenoxybutyric acid **D25**
 4-(2,4-dichlorophenoxy)butyric acid **D25**
 2-(2,4-dichlorophenoxy)ethyl hydrogen sulfate, sodium salt **D57**
 4-(2,4-dichlorophenoxy)-2-methoxy-1-nitrobenzene **C106**
 5-(2,4-dichlorophenoxy)-2-nitroanisole **C106**
 5-(2,4-dichlorophenoxy)-2-nitrobenzoic acid methyl ester **B108**
 2-[4-(2,4-dichlorophenoxy)phenoxy]propanoic acid, methyl ester **D259**
 2-(2,4-dichlorophenoxy)propanoic acid **D257**
 2-(2,4-dichlorophenoxy)propionic acid **D257**
 α -(2,4-dichlorophenoxy)propionic acid **D257**
 2,4-dichlorophenyl 3-methoxy-4-nitrophenyl ether **C106**
 dichlorophenylarsine **P98**
 1-[2-(2,4-dichlorophenyl)-2-[(2,4-dichlorophenyl)methoxy]ethyl]-1*H*-imidazole **M332**
O-(2,4-dichlorophenyl) *O,O*-diethyl ester **D167**
O-(2,4-dichlorophenyl) *O,O*-diethyl phosphorothioate **D167**
 3-(3,5-dichlorophenyl)-1,5-dimethyl-3-azabicyclo[3.1.0]hexane-2,4-dione **P277**
N-(3,5-dichlorophenyl)-1,2-dimethylcyclopropane-1,2-dicarboximide **P277**
 (*E*)-(*RS*)-1-(2,4-dichlorophenyl)-4,4-dimethyl-2-(1*H*-1,2,4-triazol-1-yl)pent-1-en-3-ol **D464**
 3-(3,4-dichlorophenyl)-1,1-dimethylurea **D579**
N'-(3,4-dichlorophenyl)-*N,N*-dimethylurea **D579**
 1-[[2-(2,4-dichlorophenyl)-1,3-dioxolan-2-yl]methyl]-1*H*-1,2,4-triazole **A256**
 \pm 3-(3,5-dichlorophenyl)-2,4-dioxo-5-methyl-5-oxazolidinecarboxylic acid, ethyl ester **C322**
 2,6-dichloro-*p*-phenylenediamine **D240**
 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl-2,4-oxazolidinedione **V23**
 1-[2-(2,4-dichlorophenyl)-4-ethyl-1,3-dioxolan-2-yl]methyl-1*H*-1,2,4-triazole **E55**
 3,4-dichlorophenyl isocyanate **D241**
 2,4-dichlorophenyl-3-(methoxycarbonyl)-4-nitrophenyl ether **B108**
 3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea **L50**
N'-(3,4-dichlorophenyl)-*N*-methoxy-*N*-methylurea **L50**
 3-(3,4-dichlorophenyl)-1-methyl-1-*n*-butylurea **N32**
 (*E*)-(\pm)- β -[(2,4-dichlorophenyl)methylene- α -(1,1-dimethylethyl)-1*H*-1,2,4-triazole-1-ethanol **D464**
 3-(3,5-dichlorophenyl) *N*-(1-methylethyl)-2,4-dioxo-1-imadazolidinecarboxamide **I62**
 2-(3,4-dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione **M120**

(RS)-3-(3,5-dichlorophenyl)-5-methyl-5-vinyl-1,3-oxazolidine-2,4-dione **V23**
 2,4-dichlorophenyl *p*-nitrophenyl ether **N112**
 1-[2-(2,4-dichlorophenyl)pentyl]-1*H*-1,2,4-triazole **P18**
 dichlorophenylphosphine **D242**
N-(3,4-dichlorophenyl)propanamide **P295**
 1-[2-(2,4-dichlorophenyl)-2-(2-propenyloxy)ethyl]-1*H*-imidazole **I4**
 1-[[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxolan-2-yl]methyl]-1*H*-1,2,4-triazole, **P306**
 1-(2,4-dichlorophenyl)-2-(3-pyridinyl)ethanone *O*-methyloxime **P360**
 di-*p*-chlorophenyl sulfone **B127**
 (±)-1-[2-(2,4-dichlorophenyl)-3-(1,1,2,2-tetrafluoroethoxy)propyl]-1*H*-1,2,4-triazole **T61**
 (RS)-2-(2,4-dichlorophenyl)-1-(1*H*-1,2,4-triazol-1-yl)hexan-2-ol **H43**
 (RS)-2-(2,4-dichlorophenyl)-3-(1*H*-1,2,4-triazol-1-yl)propyl 1,1,2,2-tetrafluoroethyl ether **T61**
 2,4-dichlorophenyltrichloromethane **D197**
 di-(*p*-chlorophenyl)trichloromethylcarbinol **D261**
 dichlorophenyltrichlorosilane **D243**
 dichloroprop **D257**
 1,1-dichloropropane **D244**
 1,2-dichloropropane **D245**
 1,3-dichloropropane **D246**
 2,2-dichloropropanoic acid, sodium salt **D20**
 dichloropropanol **D219**
 1,3-dichloropropanol **D247**
 1,3-dichloro-2-propanol **D247**
 1,3-dichloropropan-2-ol **D247**
 1,1-dichloropropan-2-one **D173**
 1,1-dichloro-2-propanone **D173**
 1,3-dichloro-2-propanone **D174**
 1,1-dichloropropene **D248**
 1,1-dichloroprop-1-ene **D248**
 1,1-dichloro-1-propene **D248**
 1,2-dichloropropene **D249**
 1,2-dichloroprop-1-ene **D249**
 1,2-dichloro-1-propene **D249**
 1,3-dichloropropene **D250**
 1,3-dichloroprop-1-ene **D250**
 2,3-dichloropropene **D251**
 2,3-dichloroprop-1-ene **D251**
 2,3-dichloro-1-propene **D251**
 1,3-dichloro-1-propene mixture with 1,2-dichloropropane **D28**
 S-(2,3-dichloro-2-propenyl) bis(1-methylethyl) carbamothioate **D69**
 dichloropropionaldehyde **P295**
 3,4'-dichloropropionaldehyde **P295**
 3',4'-dichloropropionanilide **P295**
 2,2-dichloropropionic acid **D19**
 α,α-dichloropropionic acid **D19**
 2,2-dichloropropionic acid, sodium salt **D20**
 1,1-dichloropropylene **D248**
 1,2-dichloro-1-propylene **D249**
 1,3-dichloropropylene **D250**
 2,3-dichloropropylene **D251**
 3,6-dichloro-2-pyridinecarboxylic acid **C364**
 2',4'-dichloro-2-(3-pyridyl)acetophenone *O*-methyloxime **P360**
 2,4'-dichloro-α-(pyrimidin-5-yl)benzhydrol alcohol **F4**
 Dichlorosuric **H94**
 1,2-dichlorotetrafluoroethane **D252**
 1,2-dichloro-1,1,2,2-tetrafluoroethane **D252**
 2,6-dichlorothiobenzamide **C319**
 dichlorothiocarbonyl **T140**
 dichlorotin **T159**
 dichlorotitanocene **T168**
 2,4-dichlorotoluene **D253**
 2,6-dichlorotoluene **D254**
 3,4-dichlorotoluene **D255**
 α,2-dichlorotoluene **C172**
 α,3-dichlorotoluene **C173**
 α,4-dichlorotoluene **C174**
 α,α-dichlorotoluene **B98**
m,α-dichlorotoluene **C173**
o,α-dichlorotoluene **C172**
p,α-dichlorotoluene **C174**
 dichloro-1,3,5-triazinetriene **D202**
 1,3-dichloro-*s*-triazine-2,4,6(1*H*,3*H*,5*H*)-trione **D202**
 1,3-dichloro-4-(trichloromethyl)benzene **D197**
 2,4-dichloro-1-(trichloromethyl)benzene **D197**
 3,4-dichloro-α-(trichloromethyl)benzenemethanol acetate **P215**
 4,4'-dichloro-α-(trichloromethyl)benzhydrol **D261**
 3,4-dichloro-α-(trichloromethyl)benzylalcohol acetate **P215**
 2,2'-dichlorotriethylamine **H82**
 2,4'-dichloro-α,α,α-trifluoro-4'-nitro-*m*-toluenesulfonanilide **F91**
 2,2-dichlorovinyl dimethyl phosphate **D258**
 dichloroxylenol **D256**
 2,4-dichloro-3,5-xyleneol **D256**
 dichloroprop **D257**
 dichloropropaphos **P341**
 dichlorvos **D258**
 dichlozolate **C322**
 dichromic acid (H₂Cr₂O₇), disodium salt **S61**
 dichromium sulfate **C338**
 dichromium trisulfate **C338**
 diclofop-methyl **D259**
 dicloran **D260**
 Diclotride **H94**
 dicobalt carbonyl **C371**
 dicobalt octacarbonyl **C371**
 dicofol **D261**
p,p'-dicofol **D261**
 Dicokelt **D261**
 Dicophane **D35**
 dicopper chloride trihydroxide **C441**
 dicopper oxide **C440**
 dicoumarin **D262**
 dicresyl **M324**

Dicron **D263**
 dicrotophos **D263**
 Dicumarol **D262**
 dicumyl peroxide **D264**
 di- α -cumyl peroxide **D264**
 Di-Cup **D264**
 Dicuran **C298**
 1,3-dicyanobenzene **I114**
 1,4-dicyanobenzene **T27**
m-dicyanobenzene **I114**
p-dicyanobenzene **T27**
 1,4-dicyanobutane **A49**
 β,β -dicyano-*o*-chlorostyrene **C175**
 2,3-dicyano-1,4-dithiaanthraquinone **D570**
sym-dicyanoethane **S130**
 dicyanogen **C482**
 dicyanomethane **M18**
 1,3-dicyanotetrachlorobenzene **C286**
 dicyclocarbodiimide **D267**
 dicycloheptadiene **N202**
 dicyclohexylamine **D265**
N,N-dicyclohexylamine **D265**
 dicyclohexylamine nitrite **D266**
 dicyclohexylammonium nitrite **D266**
 dicyclohexylcarbodiimide **D267**
 1,3-dicyclohexylcarbodiimide **D267**
N,N'-dicyclohexylcarbodiimide **D267**
 dicyclohexyl phthalate **D268**
N,N'-dicyclohexylthiocarbamide **D269**
 dicyclohexylthiourea **D269**
 1,3-dicyclohexyl-2-thiourea **D269**
N,N'-dicyclohexylthiourea **D269**
sym-dicyclohexylthiourea **D269**
 1,3-dicyclohexylurea **D270**
N,N'-dicyclohexylurea **D270**
 dicyclopentadiene **D271**
 dicyclopentadienyldichlorotitanium **T168**
 di-2,4-cyclopentadien-1-yliron **F32**
 dicykan **D272**
 DID47 **O55**
 didanosine **D273**
 didecyldimethylammonium chloride **D274**
 didecyl phthalate **D275**
 di-*n*-decyl phthalate **D275**
 13,19-didehydro-12,18-dihydroxysenecionan-11,16-dione
R14
 (5 α ,6 α)-7,8-didehydro-4,5-epoxy-3-ethoxy-17-methyl-
 morphinan-6-ol **E151**
 7,8-didehydro-4,5 α -epoxy-3-ethoxy-17-methylmorphinan-
 6 α -ol **E151**
 7,8-didehydro-4,5- α -epoxy-3-methoxy-17-
 methylmorphinan-6- α -ol phosphate (1:1) **C383**
 (5 α ,6 α)-7,8-didehydro-4,5-epoxy-17-methylmorphinan-3,6-
 diol **M352**
 1,6-dideoxy-1,6-di-(2-chloroethylamino)-D-mannitol
 dihydrochloride **M29**
 2',3'-dideoxyinosine **D273**
 3-[(2,6-dideoxy-3-*O*-methyl- β -D-*ribo*-hexopyranosyl)oxy]-
 5,14-dihydroxy-19-oxocard-20(22)-enolide **C536**
 di-*n*-dibutyltin oxide **D164**
 di-*p*-dimethylaminophenyl ketone **B128**
 didodecanoyl peroxide **L9**
 didodecyl phthalate **D364**
 di-*n*-dodecyl phthalate **D364**
 didodecyl 3,3'-thiopropionate **D365**
 DIDP **D355**
 Didronel **D562**
 dieldrin **D276**
 dienochlor **D277**
 diepoxybutane **D278**
 1,2,3,4-diepoxybutane **D278**
 DL-diepoxybutane **D279**
 DL-1,2,3,4-diepoxybutane **D279**
meso-diepoxybutane **D280**
meso-1,2,3,4-diepoxybutane **D280**
 (\pm)-1,2,3,4-diepoxybutane **D279**
 1,2,9,10-diepoxy-4,7-dioxadecane **E118**
 12:15,16-diepoxy-4,7,10,13-tetraoxahexadecane **T282**
 Di-estryl **S116**
 Diethacine-ethyl **D282**
 diethanolamine **D281**
N,N-diethanolamine **D281**
 diethanol methylamine **M206**
 diethanolnitrosamine **N148**
 diethatyl-ethyl **D282**
 diethenylbenzene **D580**
 7,12-diethenyl-3,8,13,17-tetramethyl-21*H*,23*H*-porphine-
 2,18-dipropanoato(4-)-*N*²¹,*N*²²,*N*²³,*N*²⁴-
 hydroxyferate(2-)-dihydrogen **H12**
 diethofencarb **D283**
 diethoxydimethylsilane **D284**
 1,1-diethoxyethane **A6**
 1,2-diethoxyethane **D285**
 2-(diethoxyphosphinothioxyloxyamino)-2-phenylace-
 tonitrile **P170**
 diethoxymethane **D286**
 1,1-diethoxymethane **D286**
 (3,4-diethoxyphenyl)carbamic acid, 1-methylethyl ester
D283
 2-(diethoxyphosphinylimino)-1,3-diethene **F109**
 diethoxyphosphorus oxychloride **D299**
 3,3-diethoxypropene **A39**
 3,3-diethoxy-1-propene **A39**
 diethquinalphion **Q5**
 diethyl acetal **A6**
 diethyl adipate **D287**
 diethylamine **D288**
N,N-diethylamine **D288**
N,N-diethylaminobenzene **D291**
 (diethylamino)ethane **T278**
 2-diethylaminoethanol **D289**
 β -(diethylamino)ethyl alcohol **D289**
 2-(diethylamino)ethylamine **D305**
N-(2-diethylaminoethyl)amine **D305**

2-(diethylamino)ethyl *p*-aminobenzoate **P273**
 1-[[2-(diethylamino)ethyl]amino]-4-(hydroxymethyl)-9*H*-thioxanthen-9-one **H84**
 5-[2-(diethylamino)ethyl]phosphorothioic acid *O,O*-diethyl ester **A156**
O-[2-(diethylamino)-6-methyl-4-pyrimidinyl] *O,O*-diethyl phosphorothioate **P209**
O-2-(diethylamino)-6-methylpyrimidin-4-yl *O,O*-diethyl phosphorothioate **P209**
O-[2-(*N,N*-diethylamino)-6-methyl-4-pyrimidinyl] *O,O*-dimethylphosphorothioate **P210**
 [4- α -[*p*-(diethylamino)phenyl]-2,4-disulfobenzylidene]-2,5-cyclohexadien-1-ylidene]diethylammonium hydroxide, inner salt, sodium salt **C386**
N-[4[[4-(diethylamino)phenyl](2,4-disulfophenyl)methylene]-2,5-cyclohexadien-1-ylidene]*N*-ethylethanaminium hydroxide, inner salt, sodium salt **C386**
 2-(diethylamino)-1-phenyl-1-propanone **D315**
 2-(diethylamino)-propiofenone **D315**
 3-diethylaminopropylamine **D290**
 diethylaniline **D291**
N,N-diethylaniline **D291**
N,N-diethylbenzenamine **D291**
 1,2-diethylbenzene **D292**
 1,3-diethylbenzene **D293**
 1,4-diethylbenzene **D294**
m-diethylbenzene **D293**
o-diethylbenzene **D292**
p-diethylbenzene **D294**
N,N'-diethyl-1,4-benzenediamine **D313**
 diethyl 1,2-benzenedicarboxylate **D314**
 diethylcarbamazine citrate **D295**
 diethylcarbamic acid, zinc salt **Z9**
 diethylcarbomodithioic acid 2-chloro-2-propenyl ester **S135**
 diethylcarbamoithioic acid, *S*-[(4-chlorophenyl)methyl] ester **T117**
 diethylcarbamoil chloride **D296**
N,N-diethylcarbamoil chloride **D296**
N,N'-diethylcarbanilide **D297**
 diethyl carbinol **M279**
 diethyl carbitol **E80**
 diethyl carbonate **D298**
 diethyl cellosolve **D285**
O,O-diethyl chloridophosphate **D299**
O,O-diethyl *O*-[2-chloro-1-(2,4-dichlorophenyl)vinyl] phosphate **C128**
*N*¹,*N*¹-diethyl-*N*⁴-(6-chloro-2-methoxy-9-acridinyl)-1,4-pentanediamine **M55**
 diethyl chlorophosphate **D299**
 diethyl chlorophosphonate **D299**
 diethyl chlorothiophosphate **D300**
O,O-diethyl chlorthiophosphate **D300**
O,O-diethyl, *O*-(α -cyanobenzylideneamino)-phosphorothioate **P170**
N,N-diethyl-1,4-diaminobenzene **D313**
N,N-diethyl-1,3-diaminopropane **D290**
O,O-diethyl *S*-(β -diethylamino)ethyl phosphorothioate **A156**
 2,2'-diethyldihexylamine **D515**
 diethyl (dimethoxythiophosphorylthio)succinate **M11**
*N*³,*N*³-diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-benzenediamine **D466**
 diethyldiphenyldichloroethane **D199**
 diethyl 1,3-dithietan-2-ylidene phosphoramidate **F109**
 diethyl dithiobis[thioformate] **D582**
O,O-diethyl dithiobis[thioformate] **D582**
 diethyldithiocarbamic acid, 2-chloroallyl ester **S135**
 diethyl dioxanthogenate **D582**
 1,4-diethylenediamine **P200**
N,N-diethylenediamine **P200**
 diethylene dioxide **D530**
 1,4-diethylene dioxide **D530**
 diethylene ether **D530**
 diethylene glycol **D301**
 diethyleneglycolamine **A127**
 diethylene glycol butyl ether acetate **B228**
 diethylene glycol diacrylate **D302**
 diethylene glycol diethyl ether **E80**
 diethylene glycol dimethyl ether **D338**
 diethylene glycol monobutyl ether **B227**
 diethylene glycol monoethyl ether acetate **E77**
 diethylene glycol monomethyl ether **M135**
 diethylene imidoxide **M353**
 diethylene oxide **T72**
 diethylene oximide **M353**
 diethylenetriamine **D303**
N,N-diethylethanamine **T278**
N,N-diethyl-1,2-ethanediamine **D305**
 diethyl ethanedioate **D312**
N,N-diethylethanolamine **D289**
 (*E*)-4,4'-(1,2-diethyl-1,2-ethenediyl)bisphenol **S116**
 diethyl ether **D304**
N,N-diethylethylenediamine **D305**
O,O-diethyl *S*-ethylmercaptoethyl phosphorodithioate **D566**
O,O-diethyl *S*-[2-(ethylsulfonyl)ethyl] phosphorothioate **D56**
O,O-diethyl *S*-[2-(ethylthio)ethyl] phosphorodithioate **D566**
O,O-diethyl *O*-2-ethylthioethyl phosphorothioate **D51**
O,O-diethyl *S*-2-ethylthioethyl phosphorothioate **D53**
O,O-diethyl *S*-[2-(ethylthio)ethyl] phosphorothioate **D53**
O,O-diethyl *O*-[2-(ethylthio)ethyl]phosphorothioate and *O,O*-diethyl *S*-[2-(ethylthio)ethyl]phosphorothioate **D49**
O,O-diethyl *S*-[(ethylthio)methyl]phosphorodithioate **P145**
 diethylformal **D286**
 diethyl hexanedioate **D287**
 di-2-ethylhexyl adipate **D514**
 di(2-ethylhexyl)phosphate **D518**
 di(2-ethylhexyl) sodium sulfosuccinate **D583**
 1,2-diethylhydrazine **D306**

N,N'-diethylhydrazine **D306**
sym-diethylhydrazine **D306**
O,O-diethyl 7-hydroxy-3,4-tetramethylenecoumarinyl phosphorothioate **C450**
O,O-diethyl *S*-isopropylcarbamoylmethyl phosphorodithioate **P342**
O,O-diethyl *O*-(2-isopropyl-6-methylpyrimidin-4-yl) phosphorothioate **D99**
 diethyl ketone **D307**
 diethylmercury **D308**
N,N-diethyl-2-methylbenzamide **D320**
N,N-diethyl-4-methylbenzamide **D321**
O,O-diethyl *O*-(4-methylcoumarin-7-yl) phosphorothioate **D309**
 diethyl 4-methyl-1,3-dithiolan-2-ylidenephosphoramidate **M56**
O,O-diethyl *S*-methyl dithiophosphate **D310**
O,O-diethyl *O*-(5-methyl-6-ethoxycarbonylpyrazolo[1,5-*a*]pyrimid-2-yl)-thionophosphate **P350**
 diethyl 3-methylpyrazol-5-yl phosphate **D311**
O,O-diethyl *O*-(4-methylsulfinyl)phenyl phosphorothioate **F23**
N,N'-diethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine **S38**
N,N-diethyl-2-(1-naphthalenyloxy)propanamide **N28**
N,N-diethyl-2-(1-naphthylloxy)propionamide **N28**
 diethyl *p*-nitrophenyl phosphate **P10**
O,O-diethyl *O*-4-nitrophenyl phosphorothioate **P13**
 diethylnitrosamine **N149**
 diethyl oxalate **D312**
O,O-diethyl *S*-(4-oxobenzotriazin-3-methyl)phosphorodithioate **A263**
O,O-diethyl *S*-[4-(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl)methyl]phosphorodithioic acid ester **A263**
 3,3'-diethylpentamethineethiacyanine iodide **D571**
 diethyl [1,2-phenylenebis(iminocarbonothioyl)]-bis[carbamate] **T137**
 diethyl 4,4'-(*o*-phenylenebis)3-thioallophanate **T137**
N,N-diethyl-*p*-phenylenediamine **D313**
O,O-diethyl *O*-(1-phenyl-1*H*-1,2,4-triazol-3-yl) phosphorothioate **T205**
 diethylphosphoric acid chloride **D299**
 diethyl phosphorochloride **D299**
 diethyl phosphorothionochloride **D300**
 diethyl phthalate **D314**
N,N-diethyl-1,3-propanediamine **D290**
 diethylpropion **D315**
 diethylpropion hydrochloride **D316**
O,O-diethyl *O*-(2-quinoxaliny) ester of phosphorothioic acid **Q5**
O,O-diethyl *O*-quinoxalin-2-yl phosphorothioate **Q5**
 α,α' -diethyl-4,4'-stilbenediol **S116**
trans-diethylstilbestrol **S116**
 diethylstilbestrol dipropionate **S117**
 diethylstilbestrol monoglucuronide **S118**
 diethyl sulfate **D317**
 diethyl sulfide **E172**
O,O-diethyl *O*-(7,8,9,10-tetrahydro-6-oxobenzo[*c*]chromen-3-yl) phosphorothioate **C450**
O,O-diethyl *O*-(7,8,9,10-tetrahydro-6-oxo-6*H*-dibenzo[*b,d*]pyran-3-yl) phosphorothioate **C450**
 3,3'-diethylthiadicyanocyanine iodide **D571**
N,N'-diethylthiocarbamide **D318**
 diethyl thioether **E172**
 diethyl thioperoxycarbonate **D582**
O,O-diethyl thiophosphorochloride **D300**
 diethyl thiophosphoryl chloride **D300**
 1,3-diethylthiourea **D318**
 1,3-diethyl-2-thiourea **D318**
N,N'-diethylthiourea **D318**
N,N-diethyl-*m*-toluamide **D319**
N,N-diethyl-*o*-toluamide **D320**
N,N-diethyl-*p*-toluamide **D321**
O,O-diethyl *O*-(3,5,6-trichloro-2-pyridyl) phosphorothioate **C313**
N,N,N'-diethyl- α,α,α -trifluoro-3,5-dinitrotoluene-2,4-diamine **D466**
 diethylzinc **D322**
 Difen **D536**
 difenacoum **D323**
 Difenex **C106**
 difenoxuron **D324**
 Difenson **C127**
 difenylin **D543**
 difenzoquat methyl sulfate **D325**
 difenzoquat metilsulfate **D325**
 diferuloylmethane **C478**
 diflubenzuron **D326**
 diflufenican **D327**
 Diflufenicanil **D327**
 diflunisal **D328**
 difluorine monoxide **O61**
 difluorine oxide **O61**
 2,4-difluoroaniline **D329**
 2,4-difluorobenzenamine **D329**
 1,1-difluoro-1-chloroethane **C191**
 difluorochloromethane **C192**
 difluorodibromomethane **D131**
 1,1-difluoro-2,2-dichloroethyl methyl ether **M138**
 difluorodichloromethane **D204**
 1,1-difluoroethane **D330**
 1,2-difluoroethane **D331**
 1,1-difluoroethene **D332**
 1,1-difluoroethylene **D332**
 difluoroformaldehyde **C80**
 2',4'-difluoro-4-hydroxy-[1,1'-biphenyl]-3-carboxylic acid **D328**
 2',4'-difluoro-4-hydroxy-3-biphenylcarboxylic acid **D328**
 4-(difluoromethoxy)- α -(1-methylethyl)benzeneacetic acid cyano(3-phenoxyphenyl)methyl ester **F43**
 1,1-difluoroperchloroethane **D333**
 5-(2,4-difluorophenyl)salicylic acid **D328**
N-(2,4-difluorophenyl)-2-[3-(trifluoromethyl)phenoxy]-3-pyridinecarboxamide **D327**

difluorotetrachloroethane **D333**
 1,1-difluorotetrachloroethane **D333**
 1,2-difluorotetrachloroethane **D334**
 (RS)-2,4'-difluoro- α -(1*H*-1,2,4-triazol-1-ylmethyl)benzhydrol alcohol **F93**
 2',4'-difluoro-2-(α,α,α -trifluoro-*m*-tolylxy)nicotinamide **D327**
 difolatan **C58**
 Digacin **D339**
 digallium trioxide **G6**
 DIGIF **B117**
 Digisidin **D335**
 Digitoxigenin tridigitoxoside **D335**
 digitoxin **D335**
 Digitphyllin **D335**
 Digitrin **D335**
N,N-diglycidylaniline **D336**
 diglycidyl ether **D337**
 diglycidyl ethylene glycol **E118**
 1,3-diglycidylxybenzene **R6**
 diglycine **I11**
 diglycol monobutyl ether acetate **B228**
 diglycol monomethyl ether **M135**
 diglykokoll **I11**
 diglyme **D338**
 digoxin **D339**
 diheptyl phthalate **D340**
 di-*n*-heptyl phthalate **D340**
 dihexyl **D585**
 di(2-hexyloxyethyl) adipate **B129**
 dihexyl phthalate **D341**
 di-*n*-hexyl phthalate **D341**
 dihydrazinebenzenesulfonic acid **O53**
 Dihydrin **D344**
 1,2-dihydroacenaphthylene **A3**
 dihydroactinidinolide **D342**
 dihydroaflatoxin B₁ **A54**
 dihydroazirene **A266**
 dihydro-1*H*-azirine **A266**
 7,11b-dihydrobenz[*b*]indeno[1,2-*d*]pyran-3,4,6a,9,10(6*H*)-pentol **H14**
 1,3-dihydrobenzo[*c*]thiophene **D343**
 3,4-dihydrochlorothiazide **H94**
 dihydrocodeine **D344**
 9,10-dihydro-8a,10a-diazoniaphenanthrene **D560**
 10,11-dihydro-5*H*-dibenz[*b,f*]azepine **I12**
 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one **N31**
 (13 α ,14 α)-14,19-dihydro-12,13-dihydroxy-20-norcrotolan-11,15-dione **M342**
 1,4-dihydro-1,4-diketophthalene **N20**
 2,3-dihydro-2,2-dimethylbenzofuranyl [(dibutylamino)thio]methylcarbamate **C83**
 2,3-dihydro-2,2-dimethyl-7-benzofuranyl 2,4-dimethyl-5-oxo-6-oxa-3-thia-2,4-diazadecanoate **F125**
 2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate **C68**
 2,3-dihydro-2,2-dimethyl-7-benzofuranyl, 2-methyl-4-(1-methylethyl)-7-oxo-8-oxa-3-thia-2,4-diazadecanoate **B30**
 10,11-dihydro-*N,N*-dimethyl-5*H*-dibenz[*b,f*]azepine-5-propanamine **I14**
 2,3-dihydro-5,6-dimethyl-1,4-dithiin, 1,1,4,4-tetraoxide **D374**
 1,2-dihydro-1,5-dimethyl-2-phenyl-3*H*-pyrazol-3-one, compound with 2,2,2-trichloro-1,1-ethanediol(1:2) **D170**
 3,7-dihydro-1,3-dimethyl-1*H*-purine-2,6-dione **T110**
 3,7-dihydro-3,7-dimethyl-1*H*-purine-2,6-dione **T109**
 3,7-dihydro-1,3-dimethyl-1*H*-purine-2,6-dione with 1,2-ethanediamine (2:1) **A147**
 2-[7-[1,3-dihydro-1,1-dimethyl-3-(4-sulfobutyl)-2*H*-benz[*e*]indolin-2-ylidene]1,3,5-heptatrienyl]-1,1-dimethyl-3-(4-sulfobutyl)-1*H*-benz[*e*]indolium, hydroxide, inner salt, sodium salt **I30**
 9,10-dihydro-9,10-dioxo-1-anthracenesulfonic acid, sodium salt **S42**
 dihydro-2,5-dioxofuran **M13**
 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid **T299**
 S-[(1,3-dihydro-1,3-dioxo-2*H*-isindol-2-yl)methyl] *O,O*-dimethyl phosphorodithioate **P153**
 5,10-dihydro-5,10-dioxonaphtho[2,3-*b*]-1,4-dithiin-2,3-dicarbonitrile **D570**
 6,7-dihydrodipyrido[1,2-*a*:2',1'-*c*]pyrazinediium **D560**
 6,7-dihydrodipyrido[1,2-*a*:2',1'-*c*]pyrazinediium, dibromide **D561**
 dihydrofumaric acid **S128**
 dihydro-2,5-furandione **S129**
 dihydro-2-(3*H*)-furanone **B288**
 dihydrogen **H96**
 dihydrogen dioxide **H103**
 dihydrogen disodium ethylenedinitrilo(tetraacetate)cuprate(2-) **C436**
 dihydrogen [[*N,N'*-1,2-ethanediylbis-[*N*-(carboxymethyl)-glycinato]](4-)-*N,N',O,O',O,N',O,N'*]cuprate(2-) **E5**
 dihydrogen selenide **H104**
 dihydrogen sulfate **S152**
 3a,12c-dihydro-8-hydroxy-6-methyl-7*H*-furo[3',2':4,5]furo-[2,3-*c*]xanthen-7-one **S114**
 (3*R*,4*S*-4,6-dihydro-8-hydroxy-3,4,5-trimethyl-6-oxo-3*H*-2-benzopyran-7-carboxylic acid **C353**
 4,5-dihydroimidazole-2(3*H*)-thione **E122**
 2,3-dihydro-1*H*-indene **I17**
 2,3-dihydro-1*H*-indene-1-one **I20**
 2,3-dihydro-1*H*-inden-5-ol **I19**
 1,3-dihydro-1*H*-inden-2-one **I21**
 3,4-dihydro-2(1*H*)-isoquinolinecarboxamidine **D36**
 3,4-dihydro-2(1*H*)-isoquinolinecarboximidamide **D36**
 1,2-dihydro-2-ketobenzisulfonazole **S1**
 S-2,3-dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl *O,O*-dimethyl phosphorodithioate **M121**
 3,12-dihydro-6-methoxy-3,3,12-trimethyl-7*H*-pyrano(2,3-*c*)acridin-7-one **A40**
 1,2-dihydro-3-methylbenz[*j*]aceanthrylene **M190**
 2,3-dihydro-2-methyl-7-benzofuranyl methylcarbamate **D43**

2,3-dihydro-2-methylbenzofuran-7-yl methylcarbamate **D43**
2,3-dihydro-4-methylfuran **D345**
dihydro-5-methyl-2(3*H*)-furanone **V3**
1,3-dihydro-1-methyl-2*H*-imidazole-2-thione **M122**
2,3-dihydro-2-methyl-1*H*-indole **M239**
(±)-2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1*H*-imidazol-2-yl]-5-ethyl-3-pyridinecarboxylic acid **I7**
2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1*H*-imidazol-2-yl]-4(or 5)-methylbenzoic acid, methyl ester **I5**
2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1*H*-imidazol-2-yl]-3-pyridinecarboxylic acid **I6**
3,7-dihydro-1-methyl-3-(2-methylpropyl)-1*H*-purine-2,6-dione **I93**
3,4-dihydro-2-methyl-4-oxo-3-*o*-tolylquinazoline **M119**
5,6-dihydro-2-methyl-*N*-phenyl-1,4-oxathlin-3-carboxamide, 4,4-dioxide **O56**
2,4-dihydro-5-methyl-2-phenyl-3*H*-pyrazol-3-one **P121**
5,5,6-dihydro-6-methyl-2*H*-pyran-2-one **P12**
2,3-dihydro-6-methyl-2-thioxo-4(1*H*)pyrimidinone **M312**
3,4-dihydronaphthalenone **T82**
3,4-dihydro-1-(2*H*)-naphthalenone **T83**
3,4-dihydro-2(1*H*)-naphthalenone **T84**
Dihydroneopine **D344**
1,2-dihydro-5-nitroacenaphthylene **N71**
1,3-dihydro-7-nitro-5-phenyl-2*H*-1,4-benzodiazepin-2-one **N67**
dihydro-1-nitroso-2,4(1*H*,3*H*)-pyrimidinedione **N150**
5,6-dihydro-1-nitrosouracil **N150**
2,3-dihydro-3-oxobenzisulfonazole **S1**
5,3,4-dihydro-4-oxobenzo-[*d*]-1,2,3-triazin-3-ylmethyl **A264**
5-(3,4-dihydro-4-oxobenzo-[*d*]-[1,2,3]-triazin-3-ylmethyl)-*O,O*-diethyl phosphorodithioate **A263**
2-(1,3-dihydro-3-oxo-2*H*-indol-2-ylidene)-1,2-dihydro-3*H*-indol-3-one **I25**
O-(1,6-dihydro-6-oxo-1-phenyl-3-pyridazinyl) *O,O*-diethyl phosphorothioate **P355**
O-(1,6-dihydro-6-oxo-1-phenylpyridazin-3-yl) *O,O*-diethyl phosphorothioate **P355**
2-(1,3-dihydro-3-oxo-5-sulfo-2*H*-indol-2-ylidene)-2,3-dihydro-3-oxo-1*H*-indole-5-sulfonic acid, disodium salt **I26**
4,5-dihydro-2-phenyl-1*H*-imidazole **P112**
dihydrophosphine oxide **P157**
2,3-dihydro-6-propyl-2-thioxo-4(1*H*)pyrimidinone **P337**
3,7-dihydro-1*H*-purine-2,6-dione **X2**
1,7-dihydro-6*H*-purine-6-thione **M63**
7,9-dihydro-1*H*-purine-2,6,8(3*H*)-trione **U14**
dihydropyran **D346**
3,4-dihydro-2*H*-pyran **D346**
Δ²-dihydropyran **D346**
3,4-dihydro-2*H*-pyran-2-carboxaldehyde **A36**
1,5-dihydro-4*H*-pyrazolo[3,4-*d*]pyrimidin-4-one **A70**
1,2-dihydro-3,6-pyridazinedione **M14**
1,2-dihydropyridazine-3,6-one **M14**
6,7-dihydropyrido [1,2-*a*:2',1'-*c*]pyrazine-5,8-diiium **D560**
dihydrosafrole **D347**
2',3'-dihydrosafrole **D347**
2,3-dihydrothiirene **E121**
2,5-dihydrothiophene 1,1-dioxide **S144**
2,3-dihydro-2-thioxo-4(1*H*)-pyrimidinone **T145**
10,11-dihydro-*N,N*,β-trimethyl-5*H*-dibenz[*b,f*]azepine-5-propanamine **T328**
1,2-dihydro-2,2,4-trimethyl-6-ethoxyquinoline **E85**
1,3-dihydroxy-9,10-anthracenedione **D348**
1,4-dihydroxy-9,10-anthracenedione **Q7**
1,8-dihydroxy-9,10-anthracenedione **D22**
2,6-dihydroxy-9,10-anthracenedione **A219**
1,3-dihydroxyanthraquinone **D348**
1,4-dihydroxyanthraquinone **Q7**
1,8-dihydroxyanthraquinone **D22**
2,6-dihydroxyanthraquinone **A219**
1,3-dihydroxybenzene **R5**
3,4-dihydroxybenzeneacrylic acid **C19**
2,7-dihydroxy-1,3,2-benzodioxabismole-5-carboxylic acid **B131**
2,4-dihydroxybenzophenone **B85**
6,7-dihydroxy-2*H*-1-benzopyran-2-one **E48**
2,5-dihydroxybiphenyl **P110**
2,6-dihydroxy-5-bis(2-chloroethyl)aminopyrimidine **B119**
dihydroxybusulfan **T195**
1,3-dihydroxybutane **B203**
1,4-dihydroxybutane **B204**
2,3-dihydroxybutane **B205**
[*R*-(*R**,*R**)]-2,3-dihydroxybutanedioate 5'α-ergotamane-3',6',18-trione (2:1) salt **E44**
2,3-dihydroxybutanedioic acid **T8**
[*R*-(*R**,*R**)]-2,3-dihydroxybutanedioic acid **T9**
2,3-dihydroxy-[*R*-(*R*',*R*')]-butanedioic acid, copper(II) salt **C444**
2,3-dihydroxybutanedioic acid, diammonium salt **A188**
(3*R*,3'*S*,5'*R*)-3,3'-dihydroxy-β,κ-caroten-6'-one **C56**
3,4-dihydroxycinnamic acid **C19**
6,7-dihydroxycoumarin **E48**
2,2'-dihydroxy-5,5'-dichlorodiphenyl sulfide **T121**
2,2'-dihydroxydiethylamine **D281**
4,4'-dihydroxydiethylstilbene **S116**
β,β'-dihydroxydiethyl sulfide **T129**
2,2'-dihydroxy-4,4'-dimethoxybenzophenone **D349**
p,p'-dihydroxydiphenylpropane **B133**
2,2'-dihydroxydipropyl ether **D555**
β,β'-dihydroxydi-*n*-propyl ether **D555**
2,2'-dihydroxydipropylnitrosamine **N151**
3,17-dihydroxyestratriene **E51**
dihydroxyestrin **E50**
1,2-dihydroxyethane **E116**
2,4-dihydroxyethylbenzene **E98**
3',6'-dihydroxyfluoran **F51**
2,2'-dihydroxy-3,3',5,5',6,6'-hexachlorophenylmethane **H41**
3,4-dihydroxy-1-[1-hydroxy-2-(methylamino)ethyl]benzene **A51**

2,2-dihydroxy-1,3-indandione **N60**
 2,2-dihydroxy-1*H*-indene-1,3(2*H*)-dione **N60**
 3',6'-dihydroxy-*spiro*[isobenzofuran-1(3*H*), 9'-[9*H*]xanthen]-3-one **F51**
 4',7-dihydroxyisoflavone **D18**
 7,4'-dihydroxyisoflavone **D18**
 3,5-dihydroxy- α -[(isopropylamino)methyl]benzyl alcohol **O33**
 2,2'-dihydroxyisopropyl ether **D555**
 dihydroxymethylfuratrizine **D350**
 3*S*,3*aS*,4*S*,4*aS*,7*S*,9*aR*,9*bR*,12*S*)-7,12-dihydroxy-3-methyl-6-methylene-2-oxoperhydro-4*a*,7-methano-9*b*,3-propeno[1,2-*b*]furan-4-carboxylic acid **G14**
 14,16-dihydroxy-3-methyl-7-oxo-*trans*-benzoxacyclotetradec-11-en-1-one **Z1**
 2,2'-dihydroxy-*N*-nitrosodiethylamine **N148**
 3,4-dihydroxyphenethylamine **D595**
 2,3-dihydroxyphenol **P363**
 dihydroxy-L-phenylalanine **L37**
 3,4-dihydroxyphenylalanine **L37**
 1-(3,5-dihydroxyphenyl)-1-hydroxy-2-(isopropylamino)ethane **O33**
 1-(3,5-dihydroxyphenyl)-2-(isopropylamino)ethanol **O33**
 1-(3,4-dihydroxyphenyl)-2-(methylamino)ethanol **A51**
 3-(3,4-dihydroxyphenyl)-2-methylaniline, L-alanine **M208**
 (2,4-dihydroxyphenyl)phenylmethanone **B85**
 3-(3,4-dihydroxyphenyl)-2-propenoic acid **C19**
 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4*H*-benzopyran-4-one **Q2**
 (\pm)-2,3-dihydroxypropanal **G23**
 (*R*)-2,3-dihydroxypropanal **G24**
 1,2-dihydroxypropane **P327**
 di(2-hydroxypropyl)nitrosamine **N151**
 3,6-dihydroxypyridazine **M14**
 2,4-dihydroxypyrimidine **U8**
d- α , β -dihydroxysuccinic acid **T9**
 2,3-dihydroxysuccinic acid, diammonium salt **A188**
 2,6-diiodo-4-cyanophenol **I59**
 diiron trisulfate **I77**
 diisobutene **T317**
 diisobutenyl ketone **P147**
 diisobutyl adipate **D351**
 diisobutylamine **D352**
 diisobutylcarbinol **D418**
 diisobutylene **T318**
 diisobutyl ketone **D353**
 diisobutyl phthalate **D354**
 diisobutylthiocarbamic acid, *S*-ethyl ester **B243**
 Diisocarb **B243**
 diisocrotyl **D419**
 4,4'-diisocyanato-3,3'-dimethoxy-1,1'-biphenyl **D379**
 4,4'-diisocyanatodiphenylmethane **M214**
 1,6-diisocyanatohexane **H55**
 1,3-diisocyanatomethylbenzene **T175**
 2,4-diisocyanato-1-methylbenzene **T176**
 1,5-diisocyanatonaphthalene **N11**
 1,3-diisocyanatotoluene **T175**
 2,6-diisocyanatotoluene **T177**
 diisodecyl phthalate **D355**
 diisooctyl((dioctylstannylene)diethio) diacetate **D522**
 diisopropanolamine **D356**
 diisopropanolnitrosamine **N151**
 diisopropoxylphosphoryl fluoride **I106**
s-diisopropylacetone **D353**
 diisopropyl adipate **D357**
 diisopropylamine **D358**
N,N-diisopropylamine **D358**
 2,6-diisopropylamino-4-methoxytriazine **P288**
 diisopropyl ether **D359**
 diisopropyl fluorophosphate **I106**
 diisopropyl fluorophosphonate **I106**
 diisopropylidene acetone **P147**
sym-diisopropylidene acetone **P147**
 2,3:4,6-di-*O*-isopropylidene-2-keto-L-gulonic acid, sodium salt **D362**
 diisopropyl ketone **D447**
N,N'-diisopropyl-6-(methylthio)-1,3,5-triazine-2,4-diamine **P289**
N,N'-diisopropyl-6-(methylthio)-1,3,5-triazine-2,4-diamine **P289**
 di-isopropyl 5-nitroisophthalate **N178**
 diisopropyl oxide **D359**
 diisopropyl perdicarbonate **D360**
 diisopropyl peroxydicarbonate **D360**
 diisopropyl peroxydiformate **D360**
 2,6-diisopropylphenol **P314**
 diisopropyl phosphofluoridate **I106**
S-*O*,*O*-diisopropylphosphorodithioate of *N*-(2-mercaptoethyl)benzenesulfonamide **B36**
 diisotridecyl phthalate **D361**
 dikegulac-sodium **D362**
 diketene **D363**
 diketene **D363**
 2,3-diketobutane **B209**
 2,5-diketohexane **H62**
 1,3-diketohydrindene **I18**
 diketone alcohol **D65**
 2,5-diketotetrahydrofuran **S129**
 dikopan **D20**
 Dilatin **C496**
 dilauroyl peroxide **L9**
 dilauryl phthalate **D364**
 dilauryl 3,3'-thiodipropionate **D365**
 dilauryl β , β' -thiopropionate **D365**
 Dilcit **I38**
 dill apiole **D366**
 Dilurgen **S77**
 dilute hydrochloric acid **H99**
 Dimecron **P154**
 dimefox **D367**
 dimefuron **D368**
 Dimelon-methyl **M209**
 Dimepax **D372**

dimepranol **D390**
dimercaprol **D369**
dimercaptol **D369**
dimercaptopropanol **D369**
2,3-dimercapto-1-propanol **D369**
dimercury dichloride **C47**
1,4-dimesyloxybutane **B195**
dimetan **D370**
dimethachlor **D371**
dimethametryn **D372**
(1 α ,2 β ,2a β ,3 α ,6 α ,6a β ,7 β ,7a α)-2,7:3,6-dimethanonaphth[2,3-
b]oxirene **E25**
dimethazone **C359**
dimethicone **D373**
Dimethicone 350 **D373**
dimethione 350 **P222**
dimethipin **D374**
dimethirimol **D375**
dimethoate **D376**
dimethoate O-analogue **O32**
dimethoate ethyl **E71**
dimethoate oxon **O32**
dimethoxane **D377**
Dimethoxon **O32**
1,2-dimethoxy-4-allylbenzene **M223**
2,4-dimethoxyaniline hydrochloride **D378**
2,4-dimethoxybenzenamine hydrochloride **D378**
1,2-dimethoxybenzene **V18**
o-dimethoxybenzene **V18**
2,5-dimethoxybenzenazo- β -naphthol **C423**
3,3'-dimethoxybenzidine 4,4'-diisocyanate **D379**
3,4-dimethoxybenzoic acid, 4-[ethyl[2-(4-methoxyphenyl)-
1-methylethyl]amino]butyl ester **M35**
3,3'-dimethoxy-[1,1'-biphenyl]-4,4'-diamine **D95**
3,3'-dimethoxy-4,4'-biphenylene diisocyanate **D379**
2,5-dimethoxy-4-chloroaniline **C193**
dimethoxy-DDT **M132**
dimethoxyethane **D381**
1,1-dimethoxyethane **D380**
1,2-dimethoxyethane **D381**
 α,β -dimethoxyethane **D381**
dimethoxymethane **D382**
dimethoxymethylphosphine oxide **D430**
1-(3,4-dimethoxyphenol)-2-propene **M223**
1-[(3,4-dimethoxyphenyl)methyl]-6,7-dimethoxy-
isoquinoline **P4**
1-[(3,4-dimethoxyphenyl)methyl]-6,7-dimethoxy-
isoquinoline hydrochloride **P5**
di(*p*-methoxyphenyl)trichloromethylmethane **M132**
dimethoxyphosphine oxide **D449**
[(dimethoxyphosphinothioyl)thio]-butanedioic acid,
diethyl ester **M11**
2-dimethoxyphosphinothioylthio-*N*-ethylacetamide **E71**
2-dimethoxyphosphinothioylthio-*N*-formyl-*N*-
methylacetamide **F105**
3-dimethoxyphosphinothioyl thiomethyl-5-methoxy-1,3,4-
thiadiazol-2(3*H*)-one **M121**
(E) 3-dimethoxyphosphinoxyloxy-*N*-methylisocrotonamide
M343
3-[(dimethoxyphosphinyl)oxy]-2-butenic acid methyl ester
M330
3-dimethoxyphosphinyloxy-*N,N*-dimethylisocrotonamide
D263
4,5-dimethoxy-6-(2-propenyl)-1,3-benzodioxole **D366**
4,7-dimethoxy-5-(2-propenyl)-1,3-benzodioxole **A230**
dimethoxystrychine **B191**
2,3-dimethoxystrychnidin-10-one **B191**
dimethoxythiophosphonyl chloride **D407**
6,7-dimethoxy-1-veratrylisoquinoline **P4**
6,7-dimethoxy-1-veratrylisoquinoline hydrochloride **P5**
dimethyl **E58**
dimethylacetal **D380**
dimethyl acetal acetaldehyde **D380**
dimethylacetamide **D383**
N,N-dimethylacetamide **D383**
dimethylacetic acid **I98**
dimethylacetone **D307**
dimethylacetone amide **D383**
dimethyl acetonitrile **I99**
dimethylacetonylcarbinol **D65**
2,4-dimethyl-6-acetoxy-1,3-dioxane **D377**
dimethylacetylene **C469**
dimethylacetylenecarbinol **M182**
dimethylacetylenylcarbinol **M182**
O,S-dimethyl acetylphosphoramidothioate **A5**
dimethyl acid phosphite **D449**
(E)-2,3-dimethylacrylic acid **T157**
trans- α,β -dimethylacrylic acid **T157**
dimethylallyl alcohol **M176**
3,3-dimethylallyl alcohol **M176**
 α,α -dimethylallyl alcohol **M178**
2-(3,3-dimethylallyl)cyclazocine **P42**
dimethylamide acetate **D383**
dimethylamidosulfonyl chloride **D393**
dimethylamine **D384**
2,4-D, dimethylamine salt **D8**
(dimethylamino)acetonitrile **D385**
2-dimethylaminoacetonitrile **D385**
4-(dimethylamino)aniline **D448**
4-dimethylaminoantipyrine **A154**
(dimethylamino)azobenzene **D386**
4-(dimethylamino)azobenzene **M320**
N,N-dimethylaminoazobenzene **D386**
4'-(dimethylamino)azobenzene-2-carboxylic acid **M304**
4-(dimethylamino)benzaldehyde **D387**

(dimethylamino)benzaldehyde **D387**
(dimethylamino)benzene **D394**
3,4-dimethylaminobenzene **D399**
N,N-dimethylaminobenzene **D394**
4-(dimethylamino)benzenecarbonal **D387**
4,4'-dimethylaminobenzophenonimide **A254**
N,N-dimethylaminocarbonyl chloride **D406**
4-dimethylamino-3-cresyl methylcarbamate **A123**
(dimethylamino)cyclohexane **D411**

N,N-dimethylaminocyclohexane **D411**
 4-(dimethylamino)-3,5-dimethylphenol methylcarbamate (ester) **M331**
 4-dimethylamino-2,3-dimethyl-1-phenyl-3-pyrazolin-5-one **A154**
 2-(dimethylamino)-5,6-dimethyl-4-pyrimidinyl dimethylcarbamate **P208**
 (dimethylamino)ethanol **D388**
 2-dimethylaminoethanol **D388**
N,N-dimethylaminoethanol **D388**
N,N-(dimethylamino)ethanol **D388**
 2-[α -(dimethylamino)ethoxy]- α -methylbenzyl]pyridine **D598**
 2-[α -(2-dimethylaminoethoxy)- α -methylbenzyl] pyridine succinate **D599**
 1-*p*- β -dimethylaminoethoxyphenyl-*trans*-1,2-diphenylbut-1-ene **T5**
 2-dimethylaminoethoxyphenylmethyl-2-picoline **D598**
 2-dimethylaminoethoxyphenylmethyl-2-picoline succinate **D599**
 β -dimethylaminoethyl alcohol **D388**
 dimethylaminoethyl methacrylate **D389**
 2-(dimethylamino)ethyl methacrylate **D389**
 2-dimethylaminoethyl methacrylate **D389**
 β -(dimethylamino)ethyl methacrylate **D389**
 2-(dimethylamino)ethyl 2-methyl-2-propenoate **D389**
 2-[(2-dimethylaminoethyl)-2-thenylamino]pyridine **M117**
 2-[(2-(dimethylamino)ethyl)-2-thenylamino] pyridine hydrochloride **M118**
 4-dimethylamino-3-methyl-1,2-diphenyl-2-propionyloxybutene(2*S*,3*R*)-form **P318**
 3-dimethylaminomethyleneaminophenylmethylcarbamate **F102**
 3-dimethylaminomethylene iminophenyl methylcarbamate **F102**
 3-dimethylaminomethyleneiminophenyl-*N*-methylcarbamate hydrochloride **F103**
N-(2'-(dimethylamino)-2'-methyl)ethylphenothiazine **P287**
 α -[2-(dimethylamino)-1-methylethyl]- α -phenyl benzenethanol propanoate ester, (2*S*,3*R*)-form **P318**
 3-[(dimethylamino)methyl]indole **G44**
 (Z)-3-(dimethylamino)-1-methyl-3-oxo-1-propenyl dimethyl phosphate **D428**
 (E)-3-(dimethylamino)-1-methyl-3-oxo-1-propenylphosphoric acid, dimethyl ester **D263**
 4-dimethylamino-3-methylphenyl methylcarbamate **A123**
 4-(dimethylamino)-1,4,4 α ,5,5 α ,6,11,12 α -octahydro-3,6,10,12,12 α -pentahydroxy-6-methyl-1,11-dioxo-2-naphthacenecarboxamide **T62**
 2-[(*p*-(dimethylamino)phenyl)azobenzoic acid **M304**
o[(*p*-(dimethylamino)phenyl)azo]benzoic acid **M304**
 [[4-(*p*-(dimethylamino)- α -phenylbenzylidene]-2,5-cyclohexadien-1-ylidene]dimethylammonium chloride **M9**
 dimethylaminophenylmethylpyrazdone **A154**
N-[4-[[4-(dimethylamino)phenyl](2-hydroxy-3,6-disulfo-1-naphthalenyl)methylene]-2,5-cyclohexadien-1-ylidene-

N-methylmethanaminium hydroxide, inner salt, monosodium salt **C389**
S,S'-[2-(dimethylamino)-1,3-propanediyl benzenesulfonothionate **B37**
 3-(dimethylamino)propanenitrile **D391**
 1-dimethylamino-2-propanol **D390**
 1-dimethylaminopropan-2-ol **D390**
 dimethylaminopropionitrile **D391**
 3-(dimethylamino)propionitrile **D391**
 β -(dimethylamino)propionitrile **D391**
 β -(*N*-dimethylamino)propionitrile **D391**
 3-dimethylaminopropylamine **D392**
 3-dimethylamino-1-propylamine **D392**
 [3-(dimethylamino)propyl]carbamic acid, propyl ester, hydrochloride **P291**
N-(3-dimethylaminopropyl)-3-chlorophenothiazine **C310**
 5-[3-(dimethylamino) propyl]-10,11-dihydro-5*H*-dibenz[*b,f*]azepine **I14**
 10-[2-(dimethylamino)propyl]phenothiazine **P287**
 10-[3-(dimethylamino)propyl]phenothiazine hydrochloride **P285**
 10-[γ -(dimethylamino)-*N*-propyl]phenothiazine hydrochloride **P285**
N-(dimethylamino)succinamic acid **D21**
 dimethylaminosulfonyl chloride **D393**
S,S'-[2-(dimethylamino)trimethylene]bis-(benzenethiosulfonate) **B37**
S,S'-2-dimethylaminotrimethylene di(benzenethiosulfonate) **B37**
N,N-dimethyl-5-amino-1,2,3-trithianyl ethanedioate **T126**
 5-dimethylamino-1,2,3-trithianyl hydrogen oxalate **T126**
 4-(dimethylamino)-3,5-xylyl-*N*-methylcarbamate **M331**
 dimethylaniline **D394**
 2,3-dimethylaniline **D395**
 2,4-dimethylaniline **D396**
 2,5-dimethylaniline **D397**
 2,6-dimethylaniline **D398**
 3,4-dimethylaniline **D399**
 3,5-dimethylaniline **D400**
N,N-dimethylaniline **D394**
N,N-dimethylaniline methiodide **P139**
 dimethylarsenic acid **C1**
 dimethylarsinic acid **C1**
 dimethylbenzanthracene **D401**
 7,12-dimethylbenz[*a*]anthracene **D401**
 9,10-dimethyl-1,2-benzanthracene **D401**
 dimethylbenz[*a*]anthracene **D401**
 2,3-dimethylbenzenamine **D395**
 2,4-dimethylbenzenamine **D396**
 2,5-dimethylbenzenamine **D397**
 2,6-dimethylbenzenamine **D398**
 3,4-dimethylbenzenamine **D399**
 3,5-dimethylbenzenamine **D400**
N,N-dimethylbenzenamine **D394**
 dimethylbenzene **X8**
 1,2-dimethylbenzene **X6**
 1,3-dimethylbenzene **X5**

1,4-dimethylbenzene **X7**
m-dimethylbenzene **X5**
o-dimethylbenzene **X6**
p-dimethylbenzene **X7**
N,N-dimethyl-1,4-benzenediamine **D448**
 dimethyl 1,2-benzenedicarboxylate **D450**
 dimethyl 1,4-benzenedicarboxylate **D459**
 α,α -dimethylbenzeneethanamine **P88**
N,N-dimethylbenzenemethanamine **D403**
 $\alpha,4$ -dimethylbenzenemethanol **D402**
 α,α -dimethylbenzenemethanol **P131**
 dimethyl benzeneorthodicarboxylate **D450**
 3,3'-dimethylbenzidine **T172**
 dimethylbenzimidazolylcobamide **C368**
 5,6-dimethylbenzimidazolylcobamide cyanide **C368**
 2,2-dimethyl-1,3-benzodioxol-4-ol methylcarbamate **B28**
 3,5-dimethylbenzoic acid 1-(1,1-dimethylethyl)-2-(4-ethylbenzoyl)hydrazide **T12**
 $\alpha,4$ -dimethylbenzyl alcohol **D402**
 α,α -dimethylbenzyl alcohol **P131**
 α,p -dimethylbenzyl alcohol **D402**
 dimethylbenzylamine **D403**
N,N-dimethylbenzylamine **D403**
 dimethylbenzyl hydroperoxide **C475**
 1-(α,α -dimethylbenzyl)-3-(4-methylphenyl)urea **D603**
 1-(α,α -dimethylbenzyl)-3-*p*-tolylurea **D603**
 6,6-dimethyl-bicyclo[3.1.1]hept-2-ene-2-carboxaldehyde **M365**
 1,1-dimethylbiguanide hydrochloride **M100**
 3,3'-dimethyl-[1,1'-biphenyl]-4,4'-diamine **T172**
 6,6'-[(3,3'-dimethyl[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis(4-amino-5-hydroxy)-1,3-naphthalenedisulfonic acid, tetrasodium salt **E190**
 3,3'-[(3,3'-dimethyl-4,4'-biphenylene)bis(azo)]bis(5-amino-4-hydroxy-2,7-naphthalenedisulfonic acid) tetrasodium salt **T366**
 1,1'-dimethyl-4,4'-bipyridinium **P11**
 3,3'-[(3,3'-dimethyl[1,1'-bisphenyl]-4,4'-diyl)bis(azo)]bis(5-amino-4-hydroxy)-2,7-naphthalenedisulfonic acid, tetrasodium salt **T366**
O,O-dimethylboldine **G15**
 1,3-dimethylbutanamine **D404**
 1,3-dimethylbutanol **M277**
 2,2-dimethylbutanone **P192**
 3,3-dimethylbutanone **P192**
 3,3-dimethyl-2-butanone **P192**
 dimethyl (Z)-butenedioate **D426**
 4,4-dimethylbutenolide **D417**
 1,3-dimethylbutyl acetate **H77**
 1,3-dimethylbutylamine **D404**
 2,4-dimethyl-6-*tert*-butylphenol **D405**
 dimethyl-1-butyryloxy-2,2,2-trichloroethylphosphonate **B224**
 dimethylcarbamic acid 1-[(dimethylamino)carbonyl]-5-methyl-1*H*-pyrazol-3-yl ester **D462**
 dimethylcarbamic acid, ester with 3-hydroxy-5,5-dimethyl-2-cyclohexen-1-one **D370**
 dimethylcarbamic acid, 3-methyl-1-(methylethyl)-1*H*-pyrazol-5-yl ester **I107**
 dimethylcarbamic chloride **D406**
N,N-dimethylcarbamidoyl chloride **D406**
 dimethylcarbomodithioic acid, potassium salt **P247**
 dimethylcarbomodithioic acid, sodium salt **S64**
 dimethylcarbamoyle chloride **D406**
 1-(dimethylcarbamoyle)-5-methylpyrazol-3-yl dimethylcarbamate **D462**
 (E)-2-dimethylcarbamoyle-1-methylvinyl dimethyl phosphate **D263**
 dimethylcarbamyl chloride **D406**
N,N-dimethylcarbamyl chloride **D406**
 2-dimethylcarbamyl-3-methyl-5-pyrazolyl dimethylcarbamate **D462**
 dimethyl carbinol **D338**
O,O-dimethylcatechol **V18**
 dimethyl cellosolve **D381**
 dimethyl 7-chlorobicyclo[3.2.0]hepta-2,6-dien-6-yl dimethylphosphate **H29**
 dimethyl chlorothionophosphate **D407**
O,O-dimethyl chlorothionophosphate **D407**
 dimethyl chlorothiophosphate **D407**
O,O-dimethyl chlorothiophosphate **D407**
 5,6-dimethylchrysene **D408**
 4,4-dimethylcrotonolactone **D417**
 dimethylcyanomethylamine **D385**
O,O-dimethyl *O*-(4-cyanophenyl) phosphorothioate **C486**
 dimethylcyclohexanamine **D411**
 1,2-dimethylcyclohexane **D409**
o-dimethylcyclohexane **D409**
 1,3-dimethylcyclohexene **D410**
 1,3-dimethyl-1-cyclohexene **D410**
N,N-dimethylcyclohexylamine **D411**
trans-1,10-dimethyl-*trans*-9-decalol **G11**
N,N-dimethyl-1,3-diaminopropane **D392**
 2,5-dimethyl-1,4-diazine **D452**
 dimethyl 1,2-dibromo-2,2-dichloroethyl phosphate **N3**
 dimethyl 1-(2,4-dichlorophenyl)-2-chlorovinyl phosphate **D460**
 dimethyldichlorosilane **D206**
 dimethyl 2,2-dichlorovinyl phosphate **D258**
 dimethyldidecylammonium chloride **D274**
 dimethyldiethoxysilane **D284**
 dimethyl diketone **B209**
 dimethyl *cis*-2-dimethylcarbamoyle-1-methylvinyl phosphate **D263**
 1,4-dimethyl-3,6-dioxo-1-heptanol **D556**
 2,6-dimethyl-1,3-dioxan-4-ol acetate **D377**
 2,6-dimethyl-*m*-dioxan-4-ol acetate **D377**
 2,4-dimethyl-*m*-dioxanyl 6-acetate **D377**
 2,2-dimethyl-1,3-dioxolane-4-methanol **S101**
N,N-dimethyldiphenylacetamide **D536**
N,N-dimethyl-2,2-diphenylacetamide **D536**
N,N-dimethyl- α,α -diphenylacetamide **D536**
 1,2-dimethyl-3,5-diphenyl-1*H*-pyrazolium methyl sulfate **D325**

dimethyl disulfide **D412**
O,O-dimethyl dithiobis(thioformate) **D463**
N,N-dimethyldithiocarbamic acid, potassium salt **P247**
N,N-dimethyldithiocarbamic acid, sodium salt **S64**
 2,4-dimethyl-1,3-dithiolane-2-carboxaldehyde *o*-[(methylamino)carbonyl] oxime **T163**
 2,4-dimethyl-1,3-dithiolane-2-carboxyaldehyde *o*-(methylcarbomoyl) oxime **T163**
O,O-dimethyldithiophosphorylbenzeneacetic acid, ethyl ester **P89**
O,O-dimethyldithiophosphorylphenylacetic acid, ethyl ester **P89**
 dimethyl dixanthogen **D463**
 dimethylenediamine **E114**
 dimethylene glycol **B205**
 dimethyleneimine **A266**
exo-1,2-*cis*-dimethyl-3,6-epoxyhexahydrophthalic anhydride **C54**
O,O-dimethyl ester, *S*-ester with *N*-formyl-2-mercapto-*N*-methylacetamide **F105**
N,N-dimethylethanolamine **D414**
 1,1-dimethylethane **I84**
 1,1-dimethylethanol **B214**
 dimethylethanolamine **D388**
N,N-dimethylethanolamine **D388**
 dimethyl ether **D413**
 dimethyl ether, chloro **C214**
 ((1,1-dimethylethoxy)methyl)-oxirane **B260**
 1,1-dimethylethylamine **B241**
N,N-dimethylethylamine **D414**
 α 1-[(1,1-dimethylethyl)amino]methyl]-4-hydroxy-1,3-benzenedimethanol **S3**
 (1,1-dimethylethyl)benzene **B247**
 dimethylethylcarbinol **M173**
 1,1-dimethylethylcyclohexane **D415**
 2-(1,1-dimethylethyl)-4,6-dimethylphenol **D405**
 (E-1,1-dimethylethyl 4-[[[(1,3-dimethyl-5-phenoxy-1*H*-pyrazol-4-yl)methylene]amino]oxy]methyl]benzoate **F21**
 1-(1,1-dimethylethyl)-3,5-dimethyl-2,4,6-trinitro-benzene **M358**
 2-(1,1-dimethylethyl)-4,6-dinitrophenol **D512**
 dimethylethylene **B216**
sym-dimethylethylene **B217**
 dimethyl *cis*-ethylenedicarboxylate **D426**
N-(1,1-dimethylethyl)-*N'*-ethyl-6-methoxy-1,3,5-triazine-2,4-diamine **T23**
N-(1,1-dimethylethyl)-*N'*-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine **T25**
 1,1-dimethylethyl hydroperoxide **B261**
N'-[5-(1,1-dimethylethyl)-3-isoxazolyl]-*N,N*-dimethylurea **I139**
O,O-dimethyl *S*-(ethylmercapto)ethyl thiophosphate **D54**
 1-(1,1-dimethylethyl)-2-methoxy-4-methyl-3,5-dinitrobenzene **M357**
 1,1-dimethylethyl methyl ketone **P192**
 4-(1,1-dimethylethyl)-*N*-(1-methylpropyl)-2,6-dinitrobenzamine **B232**
 4-(1,1-dimethylethyl)phenol **B276**
 2-[4-(1,1-dimethylethyl)phenoxy]cyclohexyl 2-propynyl sulfite **P300**
 4-[[4-(1,1-dimethylethyl)phenyl]ethoxy]quinazoline **F6**
 4-[3-[4-(1,1-dimethylethyl)phenyl]-2-methyl-propyl]-2,6-dimethylmorpholine **F20**
 (RS)-1-[3-[4-(1,1-dimethylethyl)phenyl]-2-methylpropyl]piperidine **F19**
N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-*N,N'*-dimethylurea **T13**
O,O-dimethyl *S*-(2-(ethylthio)ethyl) phosphorothiate **D54**
S-[[[(1,1-dimethylethyl)thio]methyl] *O,O*-diethyl phosphorodithioate **T22**
 1,1-dimethylethyl 3,5,5-trimethylhexaneperoxoate **B274**
 dimethyl formal **D382**
 dimethyl formaldehyde **A17**
 dimethylformamide **D416**
N,N-dimethylformamide **D416**
 dimethylformocarbithaldine **D24**
O,O-dimethyl *S*-[2-(formylmethylamino)-2-oxoethyl] phosphorodithioate **F105**
 5,5-dimethyl-2(5*H*)-furanone **D417**
N,N-dimethylglycinonitrile **D385**
 dimethylglyoxal **B209**
 2,6-dimethyl-2,5-heptadien-4-one **P147**
 2,6-dimethyl-4-heptanol **D418**
 2,6-dimethylheptan-4-one **D353**
 2,5-dimethyl-2,4-hexadiene **D419**
 1,1-dimethylhydrazine **D420**
 1,2-dimethylhydrazine **D421**
asym-dimethylhydrazine **D420**
N,N-dimethylhydrazine **D420**
N,N'-dimethylhydrazine **D421**
sym-dimethylhydrazine **D421**
unsym-dimethylhydrazine **D420**
 1,2-dimethylhydrazine dihydrochloride **D422**
N,N'-dimethylhydrazine dihydrochloride **D422**
 dimethylhydrazinium dichloride **D422**
 1,2-dimethylhydrazinium dichloride **D422**
 2-(2,2-dimethylhydrazino)-4-(5-nitro-2-furyl)thiazole **D423**
 dimethyl hydrogen phosphite **D449**
 dimethyl(2-hydroxymethyl)amine **D388**
 dimethyl(2-hydroxypropyl)amine **D390**
O,O-dimethyl-1-hydroxy-2,2,2-trichloroethyl phosphonate **T225**
 1,2-dimethylimidazole **D424**
 1,2-dimethyl-1*H*-imidazole **D424**
N,2-dimethylimidazole **D424**
 3,4-dimethyl-3*H*-imidazo[4,5-*f*]quinolin-2-amine **M45**
 3,8-dimethyl-3*H*-imidazo[4,5-*f*]quinoxalin-2-amine **M46**
N,N-dimethylimidodicarbonimidic diamide monohydrochloride **M100**
 2,3-dimethylindene **D425**
N,N-dimethyl-1*H*-indole-3-methanamine **G44**

dimethylisopropanolamine **D390**
N,N-dimethylisopropanolamine **D390**
N'-(3,4-dimethyl-5-isoxazolyl) sulfanilamide **S141**
 dimethylketal **A17**
 dimethyl ketone **A17**
 dimethyl maleate **D426**
 dimethylmercury **D427**
N,N-dimethylmethanamide **D416**
N,N-dimethylmethanamine **T303**
 dimethylmethane **P292**
 dimethyl methanephosphonate **D430**
N,N-dimethyl-*N'*-(4-methoxy-3-chlorophenyl)urea **M325**
O,O-dimethyl-*S*-(2-methoxyethylcarbamoyl
 methyl)dithiophosphate **A110**
 2,6-dimethyl-*N*-(2-methoxyethyl)chloroacetanilide **D371**
O,O-dimethyl *S*-(5-methoxy-4-oxo-4*H*-pyran-2-yl)
 phosphorothioate **E24**
 1,1-dimethyl-3-[4-(4-methoxyphenoxy)phenyl]urea **D324**
N,N-dimethyl-*N'*-[[[(methylamino)carbonyl]oxy]-
 phenylmethanimidamide monohydrochloride **F103**
N,N-dimethyl-*N'*-[3-[[[(methylamino)carbonyl]oxy]phenyl]-
 methanimidamide **F102**
 2,2-dimethyl-4-[(*N*-methylamino)carboxylato]-1,3-
 benzodioxole **B28**
O,O-dimethyl *S*-[2-(methylamino)-2-oxoethyl]
 phosphorothioate **O32**
O,O-dimethyl *S*-(*N*-methylcarbamoyl)methyl
 phosphorodithioate **D376**
O,O-dimethyl *S*-(*N*-methylcarbamoyl)methyl
 phosphorothioate **O32**
 dimethyl (*Z*)-1-methyl-2-dimethylcarbamoylviny
 lphosphate **D428**
 (1*S*)-6,6-dimethyl-2-methylenebicyclo[3.1.1] heptane
P199
 2,2-dimethyl-3-methylene-bicyclo[2.2.1]heptane **C49**
 6,6-dimethyl-2-methylenebicyclo[3.1.1]heptane **P198**
 2,2-dimethyl-3-methylenebornene **C49**
 2,3-(dimethylmethylenedioxy)-phenyl methylcarbamate
B28
 2,2-dimethyl-3-methylenenorbornane **C49**
 3,3-dimethyl-2-methylenenorcamphane **C49**
N,N-dimethyl-*N'*-[4-(1-methylethyl)phenyl]urea **I133**
N,N-dimethyl-*N'*-(2-methyl-4-[[[(methylamino)carbonyl]-
 oxy]phenyl)methanimidamide **F106**
O,O-dimethyl *S*-[2-[[1-methyl-2-(methylamino)-2-
 oxoethyl]thio]ethyl] phosphorothioate **V9**
 (*E*)-dimethyl 1-methyl-3-(methylamino)-3-oxo-1-propenyl
 phosphate **M343**
 dimethyl (*Z*)-1-methyl-2-methylcarbamoylviny lphosphate
D429
O,O-dimethyl *O*-(3-methyl-4-nitrophenyl)
 phosphorothioate **F11**
N,N-dimethyl-2-(*o*-methyl- α -phenylbenzoyloxy)ethylamine
O35
N,N-dimethyl-2-[(2-methylphenyl)phenyl-
 methoxy]ethanamine **O35**
 dimethyl methylphosphonate **D430**
 2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropane-
 carboxylic acid, 3-(2-butenyl)-2-methyl-4-oxo-2-
 cyclopenten-1-yl ester **C344**
 2,2-dimethyl-3-(2-methylpropenyl) cyclopropanecarboxylic
 acid ester with *N*-(hydroxymethyl)-1-cyclohexene-1,2-
 dicarboximide **T85**
 2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropane-
 carboxylic acid, 1,3,4,5,6,7-hexahydro-1,3-dioxo-2*H*-
 isoindol-2-yl methyl ester **T85**
 3,3-dimethyl-1-(methylthio)-2-butanone *O*-[(methylamino)-
 carbonyl]oxime **T131**
 3,3-dimethyl-1-(methylthio)butanone-*O*-(*N*-methyl-
 carbamoyl)oxime **T131**
 3,3-dimethyl-1-methylthiobutanone *O*-
 methylcarbamoyloxime **T131**
 1-(2,2-dimethyl-1-methylthiomethylpropylideneamino-
 oxy)-*N*-methylformamide **T131**
 3,5-dimethyl-4-(methylthio)phenol **D431**
 3,5-dimethyl-4-methylthiophenyl methylcarbamate
M123
 dimethylmonoethanolamine **D388**
O,O-dimethyl *S*-(morpholino-carbonylmethyl)
 phosphorodithioate **M354**
 dimethyl morpholinophosphonate **D432**
 dimethyl morpholinophosphoramidate **D432**
O,O-dimethyl *S*-[2-(4-morpholinyl)-2-oxoethyl]
 phosphorodithioate **M354**
 1,2-dimethylnaphthalene **D433**
 1,3-dimethylnaphthalene **D434**
 1,4-dimethylnaphthalene **D435**
 1,5-dimethylnaphthalene **D436**
 1,6-dimethylnaphthalene **D437**
 1,7-dimethylnaphthalene **D438**
 1,8-dimethylnaphthalene **D439**
 2,3-dimethylnaphthalene **D440**
 2,6-dimethylnaphthalene **D441**
 2,7-dimethylnaphthalene **D442**
 dimethylnitramine **D443**
 dimethylnitroamine **D443**
 1,2-dimethyl-3-nitrobenzene **N186**
 1,2-dimethyl-4-nitrobenzene **N188**
 1,3-dimethyl-2-nitrobenzene **N185**
 1,3-dimethyl-4-nitrobenzene **N187**
 2,3-dimethylnitrobenzene **N186**
 2,4-dimethyl-1-nitrobenzene **N187**
 2,6-dimethylnitrobenzene **N185**
 3,4-dimethyl-1-nitrobenzene **N188**
 dimethylnitromethane **N139**
O,O-dimethyl *O*-(4-nitrophenyl) phosphorothioate **P14**
 dimethylnitrosamine **D444**
N,N-dimethyl-4-nitrosoaniline **D445**
N,4-dimethyl-*N*-nitrosobenzenesulfonamide **M269**
 1,1'-dimethyl-*N*-nitrosodiethylamine **N152**
 2,6-dimethylnitrosomorpholine **N153**
 2,6-dimethyl-4-nitrosomorpholine **N153**
 2,6-dimethyl-*N*-nitrosomorpholine **N153**
 6,6-dimethyl-2-norpinene-2-carboxaldehyde **M365**

3,7-dimethyl-2,6-octadienal **C351**
 2,6-dimethyl-2,6-octadien-8-ol **G12**
 2,6-dimethyl-2,7-octadien-6-ol **L47**
 3,7-dimethyl-1,6-octadien-3-ol **L47**
 3,7-dimethyl-2,6-octadien-1-ol **G12**
 1-(3,7-dimethyloctyl)-1-(2-propenyl)piperidinium bromide **P206**
N,N'-dimethylol-5,5-dimethylhydantoin **D446**
 dimethylolpropene **N40**
 2,3-dimethyl-7-oxabicyclo[2,2,1]heptane-2,3-dicarboxylic anhydride **C54**
 2,4-dimethyl-3-oxapentane **D359**
 3,3-dimethyl-2-oxethanone **P211**
 dimethyl oxide **D413**
 5,5-dimethyl-3-oxocyclohex-1-enyl dimethylcarbamate **D370**
 4-[2-(3,5-dimethyl-2-oxocyclohexyl)-2-hydroxyethyl]-2,6-piperidinedione **C513**
 3-[2-(3,5-dimethyl-2-oxocyclohexyl)-2-hydroxyethyl]glutrimide **C513**
 3,3-dimethyl-7-oxo-6-phenyl-acetamido-4-thia-1-azabicyclo[3,2,0]heptane-2-carboxylic acid **B100**
 2-(2,2-dimethyl-1-oxopropyl)-1*H*-indene-1,3(2*H*)-dione **P193**
 1-[(2,5-dimethyloxyphenyl)azo]-2-naphthalenol **C423**
 dimethyl parathion **P14**
 2,4-dimethyl-3-pentanone **D447**
 2,4-dimethylpentan-3-one **D447**
 α,α -dimethylphenethylamine **P88**
 dimethylphenol **X9**
 2,4-dimethylphenol **X10**
 2,5-dimethylphenol **X11**
 3,5-dimethylphenol **X12**
 3,6-dimethylphenol **X11**
 4,6-dimethylphenol **X10**
 dimethylphenylamine **D394**
 2,3-dimethylphenylamine **D395**
 2,4-dimethylphenylamine **D396**
 2,5-dimethylphenylamine **D397**
 3,4-dimethylphenylamine **D399**
 3,5-dimethylphenylamine **D400**
N,N-dimethylphenylamine **D394**
 2-[(2,3-dimethylphenyl)amino]benzoic acid **M42**
N,N-dimethyl(phenylazo)benzenamine **D386**
N,N-dimethyl-4-phenylazobenzenamine **M320**
 4-[(2,4-dimethylphenyl)azo]-3-hydroxy-2,7-naphthalenedisulfonic acid, disodium salt **C395**
N,N-dimethyl- α -phenylbenzenacetamide **D536**
 dimethylphenylcarbinol **P131**
N'-(2,4-dimethylphenyl)-*N*-[[2,4-dimethylphenyl]-imino]methyl]-*N*-ethylmethanimidamide **A158**
 dimethyl [1,2-phenylenebis(iminocarbonothioyl)]-bis[carbamate] **T138**
 dimethyl 4,4'-(*o*-phenylene)bis(3-thioallophanate) **T138**
N,N-dimethyl-*p*-phenylenediamine **D448**
 1,1-dimethyl-2-phenylethanamine **P88**
 dimethylphenylmethanol **P131**

N-(2,6-dimethylphenyl)-2-methoxy-*N*-(2-oxo-3-oxazolidinyl)acetamide **O45**
 3,4-dimethylphenyl methylcarbamate **X16**
 3,5-dimethylphenyl methylcarbamate **X4**
N,N-dimethyl-*N'*-(phenylmethyl)-*N'*-2-pyridinyl-1,2-ethanediamine, monohydrochloride **T334**
N,N-dimethyl-2-[1-phenyl-1-(2-pyridinyl)ethoxy]ethanamine **D598**
 1,1-dimethyl-3-phenylurea **F27**
N,N-dimethyl-*N'*-phenylurea **F27**
 dimethyl phosphite **D449**
 dimethyl phosphonate **D449**
 dimethylphosphoramidocyanidic acid, ethyl ester **T2**
O,S-dimethyl phosphoramidodithioate **M111**
 dimethyl phosphorochlorodithioate **D407**
O,O-dimethyl phosphorochlorodithioate **D407**
O,O-dimethyl phosphorodithioate **A264**
 dimethyl phthalate **D450**
O,O-dimethyl *S*-phthalimidomethyl phosphorodithioate **P153**
 dimethyl polysiloxane **P222**
 dimethylpolysiloxane **D373**
 2,2-dimethylpropane **N39**
N,N-dimethyl-1,3-propanediamine **D392**
 2,2-dimethyl-1,3-propanediol **N40**
 α,α -dimethylpropargyl alcohol **M182**
 dimethyl propiolactone **P211**
 3,3-dimethyl- β -propiolactone **P211**
 2-[(1,2-dimethylpropyl)amino]-4-(ethylamino)-6-(methylthio)-*s*-triazine **D372**
N-(1,2-dimethylpropyl)-*N'*-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine **D372**
 4-(1,1-dimethylpropyl)phenol **A205**
p-1,1-dimethylpropyl)phenol **A205**
p-(α,α -dimethylpropyl)phenol **A205**
 1,1-dimethylpropynol **M182**
 1,1-dimethyl-2-propyn-1-ol **M182**
 2,3-dimethylpyrazine **D451**
 2,5-dimethylpyrazine **D452**
 2,5(*or* 2,6)-dimethylpyrazine **D453**
 2,6-dimethylpyrazine **D454**
 2,3-dimethylpyridine **L61**
 2,4-dimethylpyridine **L62**
 2,5-dimethylpyridine **L63**
 2,6-dimethylpyridine **L64**
 α,α -dimethylpyridine **L64**
 α,γ -dimethylpyridine **L62**
N,N-dimethyl-*N'*-2-pyridinyl-*N'*-(2-thienylmethyl)-1,2-ethanediamide **M117**
 5,11-dimethyl-6*H*-pyrido[4,3-*b*]carbazole **E15**
 5,11-dimethyl-6*H*-pyrido[4,3-*b*]carbazol-9-ol **H110**
 (Z)-4,6-dimethyl-2(1*H*)-pyrimidinone[1-(2-methylphenyl)ethylidene]hydrazone **F31**
 2-[[[(4,6-dimethyl-2-pyrimidinyl)amino]carbonyl]-amino]sulfonyl]benzoic acid methyl ester **S145**
N-[(4,6-dimethylpyrimidin-2-yl)aminocarboxyl]-2-methoxycarbonylbenzenesulfonamide **S145**

N'-(4,6-dimethyl-2-pyrimidinyl)sulfanilide **S133**
 2-[3-(4,6-dimethylpyrimidin-2-yl)ureidosulfonyl]benzoic acid methyl ester **S145**
 dimethylsilicone **S32**
 dimethylsiloxane **S32**
 dimethylsiloxane **D373**
 dimethylsulfamoyl chloride **D393**
N,N-dimethylsulfamoyl chloride **D393**
N,N-dimethylsulfamyl chloride **D393**
 4,6-dimethyl-2-sulfanilamidopyrimidine **S133**
 dimethyl sulfate **D455**
 dimethyl sulfide **D456**
 dimethyl sulfone **D457**
 dimethyl sulfoxide **D458**
 dimethyl terephthalate **D459**
 dimethyl *p*-terephthalate **D459**
 dimethyl 2,3,5,6-tetrachloroterephthalate **C317**
 3,5-dimethyl-1,3,5-thiadiazine-2-thione **D24**
 dimethyl *N,N'*-[thiobis[(methylimino)carbonyloxy]]-bis(ethanimidothioate) **T128**
 dimethyl thioether **D456**
 dimethyl thioperoxydicarbonate **D463**
 5-(3,3-dimethyl-1-triazeno)imidazole-4-carboxamide **D17**
 5(*or* 4)-(3,3-dimethyl-1-triazeno)-imidazole-4(*or* 5)-carboxamide **D17**
 5-(3,3-dimethyl-1-triazenyl)-1*H*-imidazole-4-carboxamide **D17**
 dimethyl 2,2,2-trichloro-1-hydroxyethylphosphonate **T225**
O,O-dimethyl *O*-2,4,5-trichlorophenyl phosphorothioate **F8**
O,O-dimethyl *O*-(3,5,6-trichloro-2-pyridyl)phosphorothioate **C314**
 2,6-dimethyl-4-tridecylmorpholine **T273**
 2,6-dimethyl-4-tridecyltetrahydro-1,4-oxazine **T273**
 1,1-dimethyl-3-(3-trifluoromethylphenyl)urea **F47**
N,N-dimethyl-*N'*-[3-trifluoromethylphenyl]urea **F47**
N-[2,4-dimethyl-5-[[[(trifluoromethyl)sulfonyl]-amino]phenyl]acetamide **M43**
 1,1-dimethyl-3-(α,α,α -trifluoro-*m*-tolyl)urea **F47**
 2,2-dimethyltrimethylene diacrylate **N41**
N,N-dimethyl-1,2,3-trithian-5-amine hydrogen oxalate **T126**
N,N-dimethyl-1,2,3-trithian-5-ylammonium hydrogen oxalate **T126**
 dimethylurea, *O,N*-cyclooctyl-*N'*,*N'*- **C532**
 dimethylvinphos **D460**
 dimethylvinylcarbinol **M178**
 dimethylvinyl chloride **C215**
 β,β -dimethylvinyl chloride **C215**
 dimethylvinylmethanol **M178**
 dimethyl viologen **P11**
 dimethyl xanthic disulfide **D463**
 1,3-dimethylxanthine **T110**
 3,7-dimethylxanthine **T109**
 Dimethyl Yellow **M320**
 dimethylzinc **D461**

N, α -dimethyl-*N*-(phenylmethyl)benzenethanamine **B86**
 Dimeticone **D373**
 dimetilan **D462**
 Dimetox **T225**
 dimexano **D463**
 Dimilin **D326**
 Dimite **C125**
 Dimiter **D326**
 Dimop **D261**
 Dinagam **F47**
 3,4,6,7-dinaphthacridine **D102**
peri-dinaphthalene **P57**
 Dinex **I133**
 dinex **C516**
 diniconazole **D464**
 dinitolmide **D465**
 dinitramine **D466**
 dinitroaminophenol **A126**
 4,6-dinitro-2-aminophenol **A126**
 4,6-dinitro-*o*-*sec*-amylphenol **D509**
 2,4-dinitroaniline **D467**
 2,6-dinitroaniline **D468**
 3,5-dinitroaniline **D469**
 2,4-dinitrobenzenamine **D467**
 2,6-dinitrobenzenamine **D468**
 3,5-dinitrobenzenamine **D469**
 1,2-dinitrobenzene **D470**
 1,3-dinitrobenzene **D471**
 1,4-dinitrobenzene **D472**
m-dinitrobenzene **D471**
o-dinitrobenzene **D470**
p-dinitrobenzene **D472**
 dinitrobenzene (mixed) **D473**
 dinitrobenzol **D473**
 1,3-dinitrobenzol **D471**
 dinitrobutylphenol **D510**
 2,4-dinitro-6-*tert*-butylphenol **D512**
 2,4-dinitro-6-*sec*-butylphenyl acetate **D511**
 4,6-dinitro-2-*sec*-butylphenyl acetate **D511**
 2,4-dinitro-6-*sec*-butylphenyl isopropylcarbonate **D504**
 1,3-dinitro-2-chlorobenzene **C195**
 2,4-dinitrochlorobenzene **C194**
 dinitrocresol **D475**
 2,6-dinitro-*p*-cresol **D474**
 4,6-dinitro-*o*-cresol **D475**
 2,4-dinitro-6-cyclohexylphenol **C516**
 2,6-dinitro-*N,N*-dipropylcumidine **I117**
 3,5-dinitro-*N,N*-dipropylsulfanilamide **O36**
 2,6-dinitro-*N,N*-dipropyl-4-(trifluoromethyl)-benzeneamine **T294**
 2,4-dinitro-*N*³,*N*³-dipropyl-6-(trifluoromethyl)-1,3-benzenediamine **P278**
 2,6-dinitro-*N*¹,*N*¹-dipropyl-4-(trifluoromethyl)-*m*-phenylenediamine **P278**
 2,4-dinitrofluorobenzene **D476**
 dinitrogen dioxide **D478**
 dinitrogen monoxide **N183**

dinitrogen pentoxide **D477**
 dinitrogen tetroxide **D478**
 dinitrogen trioxide **D479**
 3,5-dinitro-2-hydroxytoluene **D475**
 3,5-dinitro-4-hydroxytoluene **D474**
 Dinitrol **D475**
 3,5-dinitro-2-methylbenzamide **D465**
 2,6-dinitro-4-methylphenol **D474**
 4,6-dinitro-2-(1-methyl-*n*-propyl)phenol **D510**
 dinitronaphthalene **D480**
 1,3-dinitronaphthalene **D481**
 1,5-dinitronaphthalene **D482**
 1,8-dinitronaphthalene **D483**
 dinitrophenol **D484**
 2,3-dinitrophenol **D485**
 2,4-dinitrophenol **D486**
 2,5-dinitrophenol **D487**
 2,6-dinitrophenol **D488**
 3,4-dinitrophenol **D489**
 α -dinitrophenol **D486**
 δ -dinitrophenol **D489**
 2,4-dinitrophenolate sodium **D490**
 5-[(2,4-dinitrophenyl)amino]-2-(phenylamino)benzene-sulfonic acid, sodium salt **C390**
 2,4-dinitrophenyl fluoride **D476**
 2,4-dinitrophenylhydrazine **D491**
 dinitrophenylmethane **D497**
 1,6-dinitropyrene **D492**
 1,8-dinitropyrene **D493**
 dinitrosohomopiperazine **D494**
 di-*N*-nitrosopentamethylenetetramine **D495**
N,N'-dinitrosopentamethylenetetramine **D495**
 dinitrosopiperazine **D496**
N,N'-dinitrosopiperazine **D496**
 3,7-dinitroso-1,3,5,7-tetraazabicyclo[3.3.1]nonane **D495**
 3,5-dinitro-2-toluamide **D465**
 dinitrotoluene **D497**
 2,3-dinitrotoluene **D498**
 2,4-dinitrotoluene **D499**
 2,5-dinitrotoluene **D500**
 2,6-dinitrotoluene **D501**
 3,4-dinitrotoluene **D502**
 3,5-dinitrotoluene **D503**
 Dinobas **D505**
 dinobuton **D504**
 dinocap **D505**
 dinoceton **D506**
 dinonyl 1,2-benzenedicarboxylate **D508**
 2,4-dinonylphenol **D507**
 dinonyl phthalate **D508**
 di-*n*-nonyl phthalate **D508**
 Dinopec **D510**
 Dinopol NOP **D520**
 Dinoquat **P11**
 18,19-dinorpregn-4-en-20-yn-3-one, 13-ethyl-17-hydroxy-, (17 α)- **L38**
 dinosam **D509**
 dinoseb **D510**
 dinoseb acetate **D511**
 dinoterb **D512**
 1,4-dintrosopiperazine **D496**
 di-*n*-octyl adipate **D513**
 di-*sec*-octyl adipate **D514**
 dioctylamine **D515**
 di-*sec*-octylamine **D515**
 dioctylbis[(1-oxododecyl)oxy]stannane **D524**
 dioctyldichlorotin **D523**
 dioctyldi(lauryloxy)stannane **D524**
 2,2-dioctyl-1,3,2-dioxastannepin-4,7-dione **D525**
 4,4'-dioctyldiphenylamine **D516**
 dioctyloxostannane **D526**
 dioctyloxotin **D526**
 di-*sec*-octyl peroxydicarbonate **D517**
 di-*sec*-octyl phosphate **D518**
 dioctyl phthalate **D520**
 dioctyl phthalate **D519**
 di-*n*-octyl phthalate **D520**
 di-*n*-octyl *o*-phthalate **D520**
 di-*sec*-octyl phthalate **D519**
 dioctyl sodium sulfosuccinate **D583**
 dioctylstannyl dichloride **D523**
 2,2'-[(dioctylstannylene)bis(thio)]bis[acetic acid], diisooctyl ester **D522**
 dioctylstannylene maleate **D525**
 di-*n*-octyltin bis(2-ethylhexyl) mercaptoacetate **D521**
 dioctyltin bis(2-ethylhexyl thioglycolate) **D521**
 di(*n*-octyl)tin-*S,S'*-bis(isooctyl mercaptoacetate) **D522**
 dioctyltin bis(isooctyl thioglycolate) **D522**
 dioctyltin dichloride **D523**
 dioctyltin didodecanoate **D524**
 dioctyltin dilaurate **D524**
 di-*n*-octyltin dilaurate **D524**
 dioctyltin maleate **D525**
 di-*n*-octyltin maleate **D525**
 dioctyltin oxide **D526**
 di-*n*-octyltin oxide **D526**
 2,4-D(IOE) **D10**
 Diogyn **E50**
 Diogynets **E50**
 diolamine **D281**
 diolane **M275**
 Diosmol **M28**
 diothene **P224**
 dioxabenzofos **D527**
 dioxacarb **D528**
 1,4-dioxacyclohexane **D530**
 1,3-dioxacyclopentane **D532**
 2,5-dioxahexane **D381**
 1,4-dioxan-2,3-diyl-bis[*O,O*-diethylphosphorothiolothioate] **D531**
 1,3-dioxane **D529**
 1,4-dioxane **D530**
m-dioxane **D529**
p-dioxane **D530**

1,4-dioxane, *trans*-2,3-dichloro- **D208**
p-dioxane, 2,3-dichloro- **D207**
p-dioxane, *trans*-2,3-dichloro- **D208**
 2,3-*p*-dioxanedithiol *S,S*-bis[*O,O*-diethyl phosphorodithioate] **D531**
S,S'-1,4-dioxane-2,3-diyl *O,O,O',O'*-tetraethylphosphorodithioate **D531**
 3,6-dioxaoctane **D285**
 2,4-dioxapentane **D382**
 dioxathion **D531**
 dioxethylene ether **D530**
 dioxin **D110**
 Dioxitol **D301**
 [(1,4-dioxo-1,4-butanediyl)bis(oxy)]bis[tributylstannane] **T221**
 4,4'-dioxo- β -carotene **C413**
 2,4-dioxo-5-fluoropyrimidine **F79**
 2,3-dioxoindoline **I78**
 Dioxolan **S101**
 1,3-dioxolane **D532**
 α -[(1,3-dioxolan-2-ylmethoxy)imino]benzeneacetonitrile **O42**
 (Z)-1,3-dioxolan-2-ylmethoxyimino(phenyl)acetonitrile **O42**
 2-(1,3-dioxolan-2-yl)phenyl methylcarbamate **D528**
 α -(1,3-dioxolan-2-yl)phenyl methylcarbamate **D528**
 1,3-dioxonaphthalan **P173**
 2-(2,6-dioxo-3-piperidiny)-1*H*-iso-indole-1,3(2*H*)-dione **T99**
N-(2,6-dioxo-3-piperidiny)phthalamide **T99**
 2,6-dioxopurine **X2**
 dioxyanthrachinonum **D22**
 4,4'-dioxybis[4-oxobutanoic acid] **D564**
 dioxydemeton-*S*-methyl **D55**
 dioxygen **O60**
 DIPA **D356**
 Dipanol **L45**
 Diparex **T225**
 dipentane glycol **T32**
 dipentylamine **D533**
 di-*n*-pentylamine **D533**
 dipentyl 1,2-benzenedicarboxylate **D534**
 dipentyl ether **P48**
 dipentyl phthalate **D534**
 di-*n*-pentyl phthalate **D534**
 Dipet **F97**
 Diphacin **D535**
 diphacinone **D535**
 diphebutzol **P96**
 diphenadione **D535**
 diphenamid **D536**
 Diphenex **C106**
 diphenhydramine **D537**
 diphenhydramine hydrochloride **D538**
 Diphenin **P142**
 diphenyl **B113**
 2-diphenylacetyl-1,3-diketohydrindene **D535**
 diphenylacetylene **D539**
 2-(diphenylacetyl)-1,3-indandione **D535**
 2-(diphenylacetyl)indan-1,3-dione **D535**
 2-(diphenylacetyl)-1*H*-indene-1,3(2*H*)-dione **D535**
 diphenylamine **D540**
 diphenylamine chloroarsine **D541**
N,N-diphenylaniline **T335**
N,N-diphenylbenzenamine **T335**
 diphenylbenzene **T28**
 1,2-diphenylbenzene **T30**
 1,3-diphenylbenzene **T29**
 1,4-diphenylbenzene **T31**
m-diphenylbenzene **T29**
p-diphenylbenzene **T31**
 diphenyl 1,2-benzenedicarboxylate **D549**
*N*², 3-diphenyl-*N*⁴,*N*⁵-bis(trifluoromethyl)thiazolidine-2,4,5-triylidenetriamine **F40**
 Diphenyl Blue 2B **C404**
 [Z]-2-[4-(1,2-diphenyl-1-butenyl)-phenoxy]-*N,N*-dimethylethanamine **T5**
 1,5-diphenylcarbazine **D542**
 2,2'-diphenylcarbazine **D542**
N,N'-diphenylcarbazine **D542**
sym-diphenylcarbazine **D542**
 1,5-diphenylcarbohydrazide **D542**
 2,2'-diphenylcarbonic hydrazide **D542**
 2,4'-diphenyldiamine **D543**
 diphenyldiazene 1-oxide **A274**
 diphenyl diazine **A268**
 diphenyldichlorosilane **D209**
 2,2-diphenyl-*N,N*-dimethylacetamide **D536**
 [1,1'-diphenyl]-2,5-diol **P110**
 diphenylene dioxide **D106**
 diphenyleneimine **C64**
 diphenylene ketone oxide **X3**
 diphenylenemethane **F49**
 diphenylene oxide **D111**
 1,2-diphenylethene **S115**
 diphenyl ether **D544**
 1,2-diphenylethylene **S115**
 1,2-diphenylethyne **D539**
 diphenylguanidine **D545**
 1,3-diphenylguanidine **D545**
N,N'-diphenylguanidine **D545**
sym-diphenylguanidine **D545**
 5,5-diphenylhydantoin **P141**
 diphenylhydantoin sodium **P142**
 5,5-diphenylhydantoin sodium **P142**
 1,2-diphenylhydrazine **D546**
sym-diphenylhydrazine **D546**
 5,5'-diphenylimidazolidin-2,4-dione **P141**
 5,5-diphenyl-2,4-imidazolidinedione **P141**
 diphenylene **D543**
 diphenyl ketone **B70**
 diphenylmethane **D547**
 diphenylmethane 4,4'-diisocyanate **M214**
 diphenylmethanone **B70**

2-(diphenylmethoxy)-*N,N*-dimethylethanamine **D537**
 2-(diphenylmethoxy)-*N,N*-dimethylethanamine hydrochloride **D538**
 1-(diphenylmethyl)-4-methylpiperazine **C497**
 diphenylnitrosamine **N155**
 diphenyl-*N*-nitrosamine **N155**
N,N-diphenylnitrosamine **N155**
 4-diphenylol **P127**
o-diphenylol **P125**
 diphenylolpropane **B133**
 diphenylolpropane glycidyl ether **B134**
 2,5-diphenyloxazole **D548**
 diphenyl oxide **D544**
 diphenyl oxide 4,4'-sulfohydrazide **O53**
 diphenyl phthalate **D549**
N-(3,3-diphenylpropyl)- α -methylphenethylamine **P271**
 diphenyl sulfone **P134**
 diphenyl sulfoxide **P135**
N,N'-diphenylthiocarbamide **T123**
 diphenylthiocarbazone **D576**
 diphenylthiourea **T123**
sym-diphenylthiourea **T123**
 1-[diphenyl[(3-trifluoromethyl)phenyl]methyl]-1*H*-1,2,4-triazole **F81**
 diphosphoric acid, tetraethyl ester **T68**
 diphosphorus pentoxide **P163**
 diphosphorus trioxide **P167**
 dipicrylamine **D550**
 dipolyoxyethylated polypropyleneglycol ether **P218**
 dipotassium EDTA **E6**
 dipotassium hexafluorosilicate **P250**
 dipotassium monochromate **P244**
 dipotassium persulfate **P261**
 dipotassium sulfate **P264**
 dipotassium tetraiodomercurate **P266**
 Dipriran **P314**
 di-2-propenylamine **D70**
N,N-di-2-propenyl-2-propen-1-amine **T199**
 dipropetryn **D551**
 dipropionyl peroxide **D552**
 dipropylacetic acid **V8**
 dipropyl adipate **D553**
 dipropylamine **D554**
 4-(dipropylamino)-3,5-dinitrobenzenesulfonamide **O36**
 5-dipropylamino- α,α,α -trifluoro-4,6-dinitro-*o*-toluidine **P278**
 dipropyl 1,2-benzenedicarboxylate **D558**
 dipropylene glycol **D555**
 dipropylene glycol methyl ether **D556**
 dipropylene glycol monomethyl ether **D556**
 dipropyl ether **D557**
 dipropyl hexanedioate **D553**
 dipropyl isocinchomeronate **D559**
 dipropyl ketone **H25**
 dipropylmethane **H20**
 dipropyl nitrosamine **N156**
 dipropyl oxide **D557**

dipropyl phthalate **D558**
N,N-dipropyl-1-propylamine **T342**
 dipropyl pyridine-2,5-dicarboxylate **D559**
 dipropyl 2,5-pyridinedicarboxylate **D559**
 Dipsal **G38**
 dipyrido[1,2-*a*:3',2'-*d*]imidazol-2-amine **G20**
 diquat **D560**
 diquat dibromide **D561**
 Direct Blue 10 G **C405**
 Direct Brown 95 **C407**
 Direct Brown BR **P101**
 Direct Fast Brown BRL **C407**
 Direct Fast Scarlet 3B **C408**
 Direct Red 39 **C408**
 Direfon **E63**
 Diren **T203**
 Direx **D579**
 Dirimal **O36**
 Diroicide **D295**
 Disan **B36**
 Discol DFW **D583**
 Disflamoll tof **T355**
 Disflamoll TP **T337**
 Disipal **O35**
 disodium carbamodithioic acid **N1**
 disodium chromate **S56**
 disodium copper(II) EDTA **C436**
 disodium dichromate **S61**
 disodium dichromate dihydrate **S62**
 disodium dihydrogen (1-hydroxyethylidene)diphosphonate **D562**
 disodium edetate **E7**
 disodium EDTA **E7**
 disodium 3,6-endoxohexahydrophthalate **E23**
 disodium 3,6-epoxycyclohexane-1,2-dicarboxylate **E23**
 disodium 1,2-ethanediyldis(carbamodithioic acid) **N1**
 disodium *N,N'*-1,2-ethanediyldis[*N*-(carboxymethyl)glycine] **E7**
 disodium ethanol-1,1-diphosphonate **D562**
 disodium ethylenebis(dithiocarbamate) **N1**
 disodium ethylene-1,2-bisdithiocarbamate **N1**
 disodium ethylenebis(iminodiacetic acid) **E7**
 disodium [(ethylenedinitrilo)tetraacetato]calcium **E4**
 disodium (ethylenedinitrilo)tetraacetic acid **E7**
 disodium etidronate **D562**
 disodium fluorophosphate **D563**
 disodium hexafluorosilicate **S68**
 disodium hydrogen phosphate **S79**
 disodium 6-hydroxy-3-oxo-9-xanthene-*o*-benzoate **C399**
 disodium methylarsonate **D601**
 disodium monofluorophosphate **D563**
 disodium monomethylarsonate **D601**
 disodium monosulfate **S92**
 disodium monosulfide **S93**
 disodium orthophosphate **S79**
 disodium peroxodisulfate **S84**

Disodium peroxydisulfuric acid **S84**
 disodium phosphate **S79**
 disodium phosphorofluoridate **D563**
 disodium pyrosulfite **S78**
 disodium salt **S57**
 disodium selenate **S89**
 disodium selenite **S90**
 disodium selenium trioxide **S90**
 disodium sulfate **S92**
 disodium sulfide **S93**
 disodium sulfite **S94**
 disodium tetraborate **S96**
 disodium 2',4',5',7'-tetrabromofluorescein **E29**
 disoprofol **P314**
 Dispensol Printing Yellow G **C410**
 dispermine **P200**
 Disperse Orange II **A130**
 Disperse Violet 1 **D76**
 distannoxane, hexakis(2-methyl-2-phenylpropyl)- **F7**
 Distillex DS1 **T247**
 Distillex DS2 **T249**
 Distopan **H38**
 Distranevrin **C360**
 disuccinoyl peroxide **D564**
 disulfatozirconic acid **Z23**
 disulfiram **D565**
 2,2'-disulfo-4,4'-stilbenediamine **D85**
 disulfoton **D566**
 disulfoton sulfoxide **D567**
 disulfur decafluoride **D568**
 disulfur dichloride **S154**
 disulfuric acid **S153**
 Disulphine Blue **C386**
 disul-sodium **D57**
 Di-Syston **D566**
 ditalimfos **D569**
 dithallium carbonate **T102**
 dithallium sulfate **T108**
 dithallium trioxide **T107**
 dithane **M19**
 Dithane D-14 **N1**
 2,3-dithiabutane **D412**
 dithianon **D570**
 dithiazanine iodide **D571**
 dithigon **D576**
 2,2'-dithiobis(benzothiazole) **D572**
 1,1'-dithiobis(*N,N*-diethylthioformamide) **D565**
 2,5-dithiobiurea **D573**
 2,4-dithiobiuret **D574**
 dithiocarb **D575**
 dithiocarbamidohydrazine **D573**
 dithiocarbonic anhydride **C75**
 dithioethylene glycol **E59**
 dithioglycerol **D369**
 dithioglycol **E59**
 1,3-dithiolan-2-ylidene-phosphoramidic acid, diethyl ester **P151**
 1,3-dithiolan-2-ylidene propanedioic acid bis(1-methylethyl) ester **I132**
 1,3-dithiolo[4,5-*b*]quinoxaline-2-thione **T142**
 Dithion **S147**
 dithionic acid **S153**
 dithionous acid, calcium salt(1:1) **C31**
 dithiophos **S147**
 dithizone **D576**
 Ditrac **D535**
 Ditrazine **D295**
 ditridecyl 1,2-benzenedicarboxylate **D577**
 ditridecyl phthalate **D577**
 di-[tris(2-methyl-2-phenylpropyl)tin] oxide **F7**
 Ditrofon **T225**
 diundecyl 1,2-benzenedicarboxylic acid **D578**
 diundecyl phthalate **D578**
 Diurex **D579**
 Diuril **C287**
 diurobromine **T109**
 diuron **D579**
 divanadium trioxide **V15**
 divinyl **B197**
 divinylbenzene **D580**
 divinylene oxide **F123**
 divinylene sulfide **T139**
 divinylenimine **P366**
 divinyl ether **D581**
 divinyl oxide **D581**
 divinyl sulfone **V38**
 Divopan **M34**
 dixan **D582**
 dixanthogen **D582**
 DLT **D365**
 DLTP **D365**
 DMA **D383**
 DMA **D384**
 2,4-D-DMA **D8**
 DMAE **D388**
 DMAPN **D391**
 DMBA **D401**
 7,12-DMBA **D401**
 DMDM hydantoin **D446**
 DMDT **M132**
p,p'-DMDT **M132**
p,p'-DME **D33**
 DMF **D416**
 DMF (amide) **D416**
 DMH **D421**
 DMH **D422**
 DMMP **D430**
 DMN **D444**
 DMNA **D444**
 DMNM **N153**
 DMNT **D423**
 2,5-DMP **X11**
 3,5-DMP **X12**

DMPD **D448**
 DMS **D455**
 DMS **D456**
 DMSO **D458**
 DMSP **F23**
 DMTT **D24**
 DMU **D579**
 2,4-DNa **D16**
 DNAP **D509**
 DNBP **D510**
 DNC **D475**
 DNCB **C194**
 DNFB **D476**
 2,4-DNFB **D476**
 DNOC **D475**
 2,3-DNP **D485**
 2,4-DNP **D486**
 2,5-DNP **D487**
 3,4-DNP **D489**
 DNPZ **D496**
 DNPC **D474**
 2,4-DNPH **D491**
 DNPT **D495**
 2,3-DNT **D498**
 2,4-DNT **D499**
 2,6-DNT **D501**
 3,4-DNT **D502**
 3,5-DNT **D503**
 DNTBP **D512**
 docabim **C368**
cis-13-docosenamide **E46**
 (*Z*)-13-docosenamide **E46**
 docusate sodium **D583**
 1,1a,2,2,3,3a,4,5,5a,5b,6-dodecachlorooctahydro-1,3,4-metheno-1*H*-cyclobuta[*cd*]pentalene **M334**
 dodecahydrodiphenylamine **D265**
 [7*S*-(7 α ,7 α ,14 α ,14 α)]-dodecahydro-7,14-methano-2*H*,6*H*-dipyrido[1,2- α :1',2'-*e*][1,5]diazocine **S105**
 dodecanal **D584**
 dodecane **D585**
n-dodecane **D585**
 1-dodecanethiol **D586**
tert-dodecanethiol **D587**
 dodecanoic acid **L8**
 1-dodecanol **D588**
n-dodecanol **D588**
 dodecanoyl peroxide **L9**
 dodecyl alcohol **D588**
 1-dodecyl aldehyde **D584**
 dodecylbenzene **P100**
 dodecylbenzenesulfonic acid **D589**
n-dodecylbenzenesulfonic acid **D589**
 dodecylcyclohexane **D590**
n-dodecylcyclohexane **D590**
N-dodecylguanidine acetate **D594**
 dodecylguanidine monoacetate **D594**
 1-dodecylguanidium acetate **D594**
 dodecyl mercaptan **D586**
n-dodecyl mercaptan **D586**
tert-dodecyl mercaptan **D587**
 dodecylphenol **D591**
 1-dodecylpyridinium chloride **L10**
n-dodecyl sodium sulfate **S76**
tert-dodecylthiol **D587**
 dodecyltrimethylammonium bromide **D592**
n-dodecyltrimethylammonium bromide **D592**
 dodemorph acetate **D593**
 Dodene **D594**
 dodine **D594**
 dodine acetate **D594**
 Dokirin **O50**
 Dolen-pur **H34**
 Dolestan **D538**
 Dolkwal Ponceau 3R **C414**
 dolmix **H9**
 Dolobid **D328**
 Dolomide **S5**
 dolomite **C25**
 Doloxene **P319**
 Dominex **C543**
 Donax **G44**
 Donaxine **G44**
 DOP **D519**
 DOPA **L37**
 L-DOPA **L37**
 Dopaflex **L37**
 dopamine **D595**
 Dopar **L37**
 Dopaston **L37**
 Dopegyt **M208**
 Dorado **P360**
 Doratid **B153**
 Doriden **G22**
 Dormex **C479**
 Dormigan **M119**
 Dormin **M117**
 Dorvon **P231**
 Dosanex **M325**
 Dotan **C140**
 Dotycin **E47**
 Dowanol DM **M135**
 Dowanol EP **P86**
 Dowanol PM **M146**
 Dowanol PPM **D556**
 Dowanol TMat **T283**
 Dowcil 200 **C153**
 Dowco 163 **N66**
 Dowco 199 **D569**
 Dowco 453 **H5**
 Dow Corning 200 **H53**
 Dow Corning 346 **P222**
 Dow Corning 360 Medical Fluid **D373**
 Dow Corning Q7-2587 **B63**
 Dowfume **B178**

Dowicide 2 **T258**
 Dowicide b **T55**
 Dowicide 2S **T259**
 Dow Shield **C364**
 Dowtherm 209 **M147**
 Doxinate **D583**
 doxorubicin **D596**
 doxorubicin hydrochloride **D597**
 doxylamine **D598**
 doxylamine succinate **D599**
 Dozar **M118**
 Dozer **T226**
 2,4-DP **D257**
 DPA **D540**
 DPA **V8**
 DPC **D542**
 DPC **L10**
 2,4-D PGBE **D15**
 DPH **P141**
 DPNA **N156**
 DPP **D558**
 DPS **P134**
 DPX 1410 **O47**
 DPX 3674 **H69**
 Dagnet **P56**
 Drat **C238**
 Drawin **B223**
 Drawisan **F4**
 drazoxolon **D600**
 DRC 3340 **X4**
 DRC 714 **P148**
 Drepamon **T162**
 Drewamine **M353**
 Dromalic **E65**
 Dromone **D257**
 dry ice **C74**
 Dry Lightning **S137**
 DSMA **D601**
 DTBP **D150**
 DTDP **D577**
 DTIC **D17**
 Dual **M323**
 Duelor **M323**
 Dulcin **E81**
 Dumil **D326**
 Du-Min **D326**
 Duncaine **L43**
 (+)-dunomycin **D23**
 duodecane **D585**
 duodecyl alcohol **D588**
 DuPont 1179 **M126**
 DuPont 1410 **O47**
 Duracet Yellow G **C410**
 Durafur Black RC **P105**
 Duramine Blue V **C386**
 Duramine Orange G **C392**
 Duramine Orange II **C391**
 Duramine Red W **C393**
 Duramine Rhodamine B **C396**
 Duramine Sky Blue A **C387**
 Duramine Yellow AE **C390**
 Durapel A Orange G **C392**
 Durapel A Orange II **C391**
 Durapel A Red A **C397**
 Durapel A Yellow AE **C390**
 Duratint-1000 **P176**
 durene **D602**
 Durfax 60 **P228**
 Durol **D602**
 Duromine **P88**
 Duromorph **M352**
 Durophet **A193**
 Durox **H103**
 Dursban **C313**
 Du-Ter **F26**
 Dwell **E185**
 Dyacid Orange G 175% **C392**
 Dyacid Orange II 120% **C391**
 Dyacid Red 4B 400% **C396**
 Dyacid Red J 125% **C397**
 Dyacid Red W **C393**
 Dyacid Yellow A 110% **C390**
 Dye Quinoline Yellow **Q10**
 Dyfonate **F99**
 Dymid **D536**
 Dymox **A259**
 dymron **D603**
 Dynacal **C37**
 Dynamag **M6**
 Dynarect Blue 2AH **C406**
 Dynasil A **T67**
 Dyrene **A208**
 Dyrenium **T203**
 dysprosium **D604**
 Dytomol M-83 **O13**
 E₁ **E53**
 E123 **A108**
 E140 **C252**
 E142 **C389**
 E162 **B25**
 E162 **B107**
 E202 **P263**
 E236 **F104**
 E249 **P258**
 E252 **P257**
 E321 **B245**
 E412 **G51**
 E414 **G53**
 E422 **G25**
 E432 **P227**
 E433 **P230**
 E525 **P254**
 E924 **P241**
 EA **E90**

Eagle **G18**
 Easeptol **E158**
 Eau Grison **C42**
 Ebernal **V22**
 Ebernal Ritardo **V22**
 L-eburnamonine **V22**
 (3 α ,16 α)-eburnamenin-14(15*H*)-one **V22**
 l-eburnamonine **V22**
 (-)-eburnamonine **V22**
 E.C. 3.4.22.2 **P3**
 E.C. 3.4.4.10 **P3**
 Ecatin **T134**
 ecdysone **E1**
 β -ecdysterone **E1**
 Echlomezol **E185**
 Eclipse **F17**
 Econochlor **C114**
 ecothal **T108**
 ECP **D167**
 Ectoral **F8**
 Ectrin **F28**
 Eda **E114**
 EDB **D132**
 EDC **D211**
 EDDP **E2**
 edetamine **E4**
 edetate calcium **E4**
 edetate dipotassium **E6**
 edetate disodium **E7**
 edetate sodium **E8**
 edetate trisodium **E9**
 edetic acid **E3**
 Edge **E56**
 Edicol **G51**
 Edicol FD&C Blue No.1 Lake **C411**
 Edicol Supra Green BS **C389**
 edifenphos **E2**
 editempa **E11**
 EDP **P150**
 EDPA **E11**
 EDTA **E3**
 EDTA calcium disodium salt **E4**
 EDTA copper complex **E5**
 EDTA dipotassium salt **E6**
 EDTA disodium salt **E7**
 EDTA tetrasodium salt **E8**
 EDTA trisodium salt **E9**
 EDTA zinc salt **E10**
 EDTF **E11**
 EDTMP **E11**
 EDTPA **E11**
 EE Solvent **E76**
 EFH **E124**
 Efosite Al **F108**
 Efoxon **P11**
 Efudex **F79**
 Efuzin **D594**

EGDN **E115**
 EGEE **E76**
 Egitol **H38**
 eglinazine-ethyl **E12**
 EGME **M134**
 EGMME **M134**
 EHDP **E183**
 Ehrlich's reagent **D387**
 EI 47031 **P151**
 eicosanoic acid **E13**
 2,4,6,8,10,12,14,16,18-eicosanonaene-1,20-dione, 1,20-bis(4-hydroxy-1,2,2-trimethylcyclopentyl)-4,8,13,17-tetramethyl-, (1*R*,1*R*,4*S*,4*S*)-(all-*E*)- **C57**
 5,8,11,14-eicosatetraenoic acid **A231**
 Eka-caesium **F110**
 Ekamet **E186**
 Ekatin **T134**
 Ekatin F **M354**
 Ekatin M **M354**
 Ekatin TD **D566**
 Ekksugoni **C106**
 Ektafos **D263**
 Ektasolve EP **P316**
 EL-103 **T13**
 EL-119 **O36**
 EL-222 **F4**
 EL-291 **T272**
 EL-5000 **F89**
 Elafos **C313**
 elaidic acid **O30**
 elaldehyde **P9**
 Elam **P295**
 elayl **E113**
 Eldecort **H95**
 eldopal **L37**
 Eldopaque **H107**
 Eldoquin **H107**
 Electrox **Z12**
 Elegas **S151**
 β -elemene **E14**
 Elicide **T133**
 ellipticine **E15**
 Eloxyl **B83**
 Elsan **P89**
 Eltarin **C63**
 Eltren **L10**
 Elvanol **P234**
 Emalex NN-7 **L7**
 Emanicil **S134**
 Embanox **P332**
 Embanox **B244**
 Embark **M43**
 EMC **E143**
 emepronium bromide **E16**
 Emerald Green **C431**
 Emerest 2301 **M270**
 Emerest 2801 **M270**

Emery 2310 **M270**
 emetine dihydrochloride **E17**
 emetine hydrochloride **E17**
 Emgel **E47**
 Emjel 200 **S110**
 Emka DDBSA **D589**
 Emkanol **E76**
 emodin **E18**
 Empical LX28 **S76**
 EMS **E146**
 Emulgen 6910 **P228**
 Emulgum 200 **G51**
 Emulson CAL **C32**
 E-Mycin **E47**
 enanthal **H19**
 enanthaldehyde **H19**
 enanthic acid **H22**
 enassay zinc dust **Z2**
 E306 (natural) **T169**
 Enavid **E28**
 ENB **E138**
 ENC **E157**
 End **E19**
 End **E20**
 Endocide **E24**
 Endomozal **M11**
 endosulfan **E19**
 β -endosulfan **E20**
 endosulfan cyclic sulfate **E21**
 endosulfan sulfate **E21**
 endothal **E22**
 endothall **E22**
 endothall sodium **E23**
 endothal sodium **E23**
 endothion **E24**
 Endotox **E20**
 Endotox **E19**
 Endoxan **C529**
 3,6-endoxohexahydrophthalic acid **E22**
 Endrical **E25**
 endrin **E25**
 endrin aldehyde **E26**
 Endrix **E25**
 Endrocide **C448**
 EndSpray **F26**
 enflurane **E27**
 enheptin **A141**
 enhexymal **H76**
 enhydroxynorprogesterone **N204**
 Enide **D536**
 Enidrel **N205**
 Enilconazole **I4**
 Enolofos **C128**
 enol-pterin **P345**
 Enorit **T137**
 Enorit Super **T138**
 Enovid **E28**

ENT 133 **R18**
 ENT 14250 **P204**
 ENT 154 **D475**
 ENT 16225 **D276**
 ENT 16519 **A232**
 ENT 19244 **I101**
 ENT 21040 **M223**
 ENT 24725 **D370**
 ENT 25585 **P77**
 ENT 25612 **E150**
 ENT 25644 **F1**
 ENT 25734 **M311**
 ENT 25830 **P151**
 ENT 26316 **A229**
 ENT 27305 **F106**
 ENT 27566 **F103**
 ENT 375 **E126**
 ENT 50324 **A266**
 ENT 50882 **H58**
 ENT 7543 **P353**
 ENT 27699Ge **P210**
 Entusil **S141**
 ENU **N158**
 Envert **D257**
 Enviro-S **D458**
 eosin **E29**
 Eosin Yellowish **E29**
 EP 475 **D59**
 Epal 6 **H65**
 Epal 8 **O13**
 Epatec **K10**
 E600 (pesticide) **P10**
 ephedrine **E30**
 (1R,2S)-(-)-ephedrine **E30**
 ephedrine sulfate **E31**
 Epibenzalin **N67**
 epibloc **C265**
 epibromohydrin **E32**
 epichlorohydrin **E33**
 (DL)- α -epichlorohydrin **E33**
 epiestradiol **E51**
 epifluorohydrin **E34**
 Epifrin **A51**
 Epigon **P56**
 epihydrin alcohol **G28**
 epihydrin aldehyde **G27**
 3,17-epihydroxyestratriene **E50**
 Epilim **S100**
 epinephrine **A51**
 D-epinephrine **A50**
 Epirez 501 **B259**
 EPN **E35**
 E200 (polyglycol) **P225**
 Eporal **S146**
 1,2-epoxy-3-allyloxypropane **A84**
 1,4-epoxy-1,3-butadiene **F123**
 1,2-epoxybutane **E36**

1,2-epoxy-3-chloropropane **E33**
 3,6-epoxycyclohexane-1,2-dicarboxylic acid **E22**
 1,2-epoxycyclopentane **O43**
 1,2-epoxy-4-epoxyethylcyclohexane **V32**
 epoxyethane **E120**
 1,2-epoxyethane **E120**
 (epoxyethyl)benzene **S127**
 1-epoxyethyl-3,4-epoxycyclohexane **V32**
 3-(epoxyethyl)-7-oxabicyclo[4.1.0]heptane **V32**
 1,2-epoxy-3-fluoropropane **E34**
 epoxyheptachlor **H16**
 1,2-epoxyhexadecane **E37**
 1,2-epoxyhexane **E38**
 4,7-epoxyisobenzofuran-1,3-dione, hexahydro-3a,7a-dimethyl-(3a,α,4β,7β,7aα) **C54**
 1,2-epoxy-3-isopropoxypropane **G30**
 1,8-epoxy-*p*-menthane **C343**
 4,5α-epoxy-3-methoxy-17-methyl-morphinan-6α-ol **D344**
 1,2-epoxy-3-methoxypropane **G32**
 1,2-epoxy-3-(2-methylphenoxy)propane **C461**
 1,2-epoxy-3-(*p*-nitrophenoxy)propane **G33**
 2,3-epoxy-1-(*p*-nitrophenoxy)propane **G33**
 1,2-epoxyoctane **E39**
 1,2-epoxy-*n*-octane **E39**
 1,2-epoxy-3-phenoxypropane **G35**
 1,2-epoxy-1-phenylethane **S127**
 2,3-epoxy-1-propanal **G27**
 1,2-epoxypropane **P330**
 1,3-epoxypropane **T309**
 2,3-epoxy-1-propanol acrylate **G29**
 2,3-epoxy-1-propanol methacrylate **G31**
 2,3-epoxy-1-propanol oleate **G34**
 2,3-epoxypropionaldehyde **G27**
 (2,3-epoxypropoxy)benzene **G35**
 1-(2,3-epoxypropoxy)butane **B259**
 1-(2,3-epoxypropoxy)-2-methylbenzene **C461**
 2,3-epoxypropyl acrylate **G29**
 2,3-epoxypropyl butyl ether **B259**
 2,3-epoxypropyl isopropyl ether **G30**
 2,3-epoxypropyl methacrylate **G31**
 2,3-epoxypropyl methyl ether **G32**
 2,3-epoxypropyl 4-nitrophenyl ether **G33**
 2,3-epoxypropyl oleate **G34**
 2,3-epoxypropyl phenyl ether **G35**
 epoxystyrene **S127**
 1,2-epoxy-3-(tolylxy)propane **C460**
 1,2-epoxy-4,4,4-trichlorobutane **T245**
 (-)-(1*S*,3*S*,5*R*,6*R*,7*S*,8*S*)-6,7-epoxy-3-[(*S*)-tropoyloxy]tropate **H122**
 Eprazin **P348**
 Eptam **E40**
 EPTC **E40**
 equilin **E41**
 Erade **Q11**
 Eradex **T142**
 Eradic Corbeaux **C109**

Eradic-Taupe **C109**
 Erbifos **M323**
 erbon **T261**
 Ercal **E44**
 ergocalciferol **E42**
 Ergomar **E44**
 (3β,22*E*)-ergosta-5,7,22-trien-3-ol **E43**
 ergosterin **E43**
 ergosterol **E43**
 ergotamine tartrate **E44**
 Ergotartrate **E44**
 Erinitrit **S81**
 erionite **E45**
 Eritox **M343**
 Erthro **E47**
 erucamide **E46**
 erucyl amide **E46**
 ERYC **E47**
 Ery Derm **E47**
 Erysan **C142**
 Ery-Tab **E47**
 erythritol anhydride **D278**
 erythritol anhydride **D280**
 Erythromid **E47**
 erythromycin **E47**
 erythrotin **C368**
 Erzoferro **I72**
 ES 100 **T67**
 ES 28 **T67**
 Esantene **I38**
 Esbrite **P231**
 Escal **I62**
 Escort **M328**
 escriner **P178**
 esculetin **E48**
 eserine salicylate **P179**
 eserolein **P178**
 esfenvalerate **E49**
 Esidrex **H94**
 Esperox 10 **B271**
 Esperox 31M **B273**
 E-Z Spread **C37**
 essence of mirbane **N82**
 essence of Niobe **E99**
 essential oils, rosin **R17**
 essential oils, turpentine **T374**
 Estilbin **S117**
 Estinerval **P64**
 Estinyl **E66**
 Estomycin **N38**
 Estone Yellow GN **C410**
 Estonmite **C127**
 estostep **N207**
 Estrace **E50**
 estradiol **E50**
 17α-estradiol **E51**
 α-estradiol **E51**

β -estradiol **E50**
 estradiol mustard **E52**
 estradiol phosphate polymer **P223**
 Estradurin **P223**
 estragol **A75**
 estragole **A75**
 1,3,5,7-estratetraen-3-ol-17-one **E41**
 (17 α)-estra-1,3,5(10)-triene-3,17-diol **E51**
 (17 β)-estra-1,3,5(10)-triene-3,17-diol **E50**
 (17 β)-estra-1,3,5(10)-triene-3,17-diol, bis[4-[bis(2-chloroethyl)amino]benzeneacetate] **E52**
 estra-1,3,5(10)-triene-3,17 β -diol, bis[(4-(bis(2-chloroethyl-amino)phenyl)acetate] **E52**
 (17 β)-estra-1,3,5(10)-triene-3,17-diol polymer with phosphoric acid **P223**
 (16 α ,17 β)-estra-1,3,5(10)-triene-3,16,17-triol **O25**
 1,3,5-estratrien-3-ol-17-one **E53**
 Estriol **O25**
 16 α ,17 β -estriol **O25**
 estrone **E53**
 E307 (synthetic) **T169**
 etacelasil **E54**
 etaconazole **E55**
 Etalene **F11**
 etalontin **N207**
 Etanyde **C535**
 ETH 560 **E70**
 ethal **C102**
 ethalfluralin **E56**
 ethametsulfuron-methyl **E57**
 Ethaminal **P45**
 Ethana **T247**
 ethanal **A7**
 ethanal oxime **A9**
 ethanamide **A10**
 ethanamine **E90**
 ethanamine, *N*-ethyl- **D288**
 ethanaminium, 2-(aminocarbonyl)oxy]-*N*, *N*,*N*-trimethyl-, chloride **C60**
 ethanaminium, 2-hydroxy-*N*,*N*,*N*-trimethyl-, 2-hydroxybenzoic acid salt (1:1) **C327**
N,*N'*-1,2-ethandiylbis[*N*-(carboxymethyl)glycine] trisodium salt **E9**
 1,2-ethandiyl 2-methyl-2-propenoate **E119**
 Ethane **D505**
 ethane **E58**
 ethanecarboxylic acid **P310**
 ethanedial **G39**
 1,2-ethanediamine **E114**
 1,2-ethanediamine-*N*,*N*-bis(phenylmethyl)- **B45**
 1,2-ethanedicarboxylic acid **S128**
 ethanedinitrile **C482**
 ethanedioic acid **O46**
 ethanedioic acid, copper(2+) salt (1:1), hemihydrate **C439**
 ethanedioic acid, diammonium salt, ammonium oxalate **D94**
 ethane-1,2-diol **E116**
 1,2-ethanediol **E116**
 1,2-ethanediol diglycidyl ether **E118**
 1,2-ethanediol dimethacrylate **E119**
 1,2-ethanediol dinitrate **E115**
 1,2-ethanediol monoacetate **E117**
 ethane-1,2-dione **G39**
 1,2-ethanedione **G39**
 ethanedithiol **E59**
 1,2-ethanedithiol **E59**
 [[1,2-ethanediyibis(carbamodithioato)] (2-)]manganese mixture with [[1,2-ethanediyibis(carbamodithioato)] (2-)]zinc **M19**
 [[1,2-ethanediyibis(carbamodithioato)] (2-)]-manganese **M21**
 [[1,2-ethanediyibis(carbamodithioato)] (2-)]zinc **Z18**
N,*N'*-1,2-ethanediyibis[*N*-(carboxymethyl)glycine]-tetrasodium salt **E8**
 [1,2-ethanediyibis[nitrilobis(methylene)]] tetrakis (phosphonic acid) **E11**
 1,2-ethanediyibis(oxy-2,1-ethanediyl 2-propenoate) **T281**
 2,2'-[1,2-ethanediyibis(oxyethylene)] bisoxirane **E118**
 ethane-1-hydroxy-1,1-diphosphonic acid **E183**
 ethanenitrile **A20**
 ethane pentachloride **P28**
 ethaneperoxoic acid **P51**
 ethaneperoxoic acid, 1,1-dimethyl ester **B270**
 ethane, tetrachlorodifluoro- **D334**
 ethanethioamide **T115**
 ethanethioic acid **T116**
 ethanethiol **E60**
 ethanethiolic acid **T116**
 ethanimidothioic acid, 2-(dimethylamino)-*N*-[[[(methylamino)carbonyl]oxy]-2-oxo-, methyl ester **O47**
 ethanimium, 2-hydroxy-*N*,*N*,*N*-trimethyl- **C326**
 ethanoic acid **A12**
 ethanoic acid, ammonium salt **A162**
 ethanoic acid, vinyl ester **V26**
 ethanoic anhydride **A13**
 ethanol **E61**
 ethanolamine **E62**
 ethanol, 2-butoxy-, acetate **B229**
 ethanol, 2-(diethylamino)- **D289**
 ethanol, 2,2'-[1,2-ethanediyibis(oxy)]bis- **T280**
 ethanolhydrazine **H91**
 ethanol, 2,2'-oxybis- **D301**
 Ethanox **E68**
 ethanoyl bromide **A24**
 ethanoyl chloride **A25**
 Ethazole **E185**
 ethenal, homopolymer **P234**
 ethene **E113**
 2,2'-(1,2-ethenediyl)bis[5-aminobenzenesulfonic acid] **D85**
 1,1'-(1,2-ethenediyl)bisbenzene **S115**
N,*N'*-1,2-ethenediyibis[*N*-(carboxymethyl)glycine] **E3**
 1,1'-[1,2-ethenediyibis(oxy)]bisbutane **D138**
 ethene homopolymer **P224**

ethene oxide **E120**
 ethenol **V27**
 ethenone **K8**
 ethenyl acetate **V26**
 ethenylbenzene **S126**
 ethenylbenzene, homopolymer **P231**
 5-ethenylbicyclo[2.2.1]hept-2-ene **V34**
 ethenyl butanoate **V29**
 4-ethenyl-1-cyclohexene **V31**
 5-ethenyl-6-(β -D-glucopyranosyloxy)-5,6-dihydro-1*H*,3*H*-pyrano[3,4-*c*]pyran-1-one **G10**
 ethenylmethylbenzene **M306**
 5-ethenyl-2-methylpyridine **M319**
 1-(ethenyloxy)butane **B280**
 ethenyloxyethene **D581**
 1-(ethenyloxy)-2-methylpropane **I96**
 4-ethenylpyridine **V36**
 1-ethenyl-2-pyrrolidinone **V37**
 1-ethenyl-2-pyrrolidinone polymers **P236**
 ethephon **E63**
 ether cyanatus **P312**
 ethide **D232**
 ethidimuron **E64**
 ethidium bromide **E65**
 ethine **A26**
 ethinodiol diacetate **E182**
 ethinyloestradiol **E66**
 ethinyl trichloride **T249**
 ethiofencarb **E67**
 ethion **E68**
 ethionamide **E69**
 ethirimol **E70**
 ethoate-methyl **E71**
 ethofumesate **E72**
 ethoheptazine **E73**
 ethohexadiol **E126**
 ethol **C102**
 Ethone **T286**
 Ethopaz **E68**
 Ethoprop **E74**
 ethoprophos **E74**
 4-ethoxyacetanilide **P58**
 2-ethoxyaniline **P71**
 4-ethoxyaniline **P72**
 4-ethoxy-benzenamine **P72**
 ethoxybenzene **P73**
 7-ethoxy-2*H*-1-benzopyran-2-one **E75**
 1-ethoxybutane **B257**
 3-ethoxycarbonylaminophenyl-*N*-phenylcarbamate **D59**
S-[α -(ethoxycarbonyl)benzyl] *O,O*-dimethyl phosphorodithioate **P89**
 ethoxycarbonylethylene **E89**
 (ethoxycarbonyl)methyl bromide **E102**
S-[*N*-ethoxycarbonyl-*N*-methylcarbamoylmethyl] *O,O*-diethyl phosphorodithioate **M37**
O-6-(ethoxycarbonyl)-5-methylpyrazolo[1,5-*a*]pyrimidin-2-yl *O,O*-diethyl phosphorothioate **P350**
 3-(ethoxycarbonyl)phenol **E137**
 4-(ethoxycarbonyl)phenol **E158**
 7-ethoxycoumarin **E75**
 2-ethoxy-2,3-dihydro-3,3-dimethyl-5-benzofuranol methanesulfonate **E72**
 (2-ethoxy-2,3-dihydro-3,3-dimethylbenzofuran-5-yl) methanesulfonate **E72**
 6-ethoxy-1,2-dihydro-2,2,4-trimethylquinoline **E85**
 ethoxyethane **D304**
 2-ethoxyethanol **E76**
 1-ethoxy-1-ethanol acetate **E78**
 2-ethoxyethanol acetate **E79**
 ethoxyethene **E181**
 2-(2-ethoxyethoxy)ethanol acetate **E77**
 1-ethoxyethyl acetate **E78**
 2-ethoxyethyl acetate **E79**
 β -ethoxyethyl acetate **E79**
 2-ethoxyethyl alcohol **E76**
 2-ethoxyethyl 2-[4-[[3-chloro-5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy]propanoate **H5**
 2-ethoxyethyl ether **E80**
 2-ethoxyethyl ethyl ether **D285**
O-(6-ethoxy-2-ethyl-4-pyrimidinyl) *O,O*-dimethyl phosphorothioate **E186**
O-(6-ethoxy-2-ethyl pyrimidin-4-yl) *O,O*-dimethyl phosphorothioate **E186**
 \pm -(*EZ*)-2-(1-ethoxyiminobutyl)-5-[(2-ethylthio) propyl]-3-hydroxycyclohex-2-enone **S25**
 ethoxylated sorbitan monooleate **P230**
 ethoxylated sorbitan monopalmitate **P228**
 ethoxymethane **E147**
 2-[[ethoxy[(1-methylethyl)amino]phosphinothioyl]oxy] benzoic acid, 1-methylethyl ester **I103**
 ethoxymethyl ethyl ether **D286**
 6-ethoxy-2-methyl-3-oxo-7-oxa-5-thia-2-aza-6-phosphanonanoic acid, ethyl ester, 6-sulfide **M37**
N-(4-ethoxy-3-nitrophenyl)acetamide **N72**
 7-ethoxy-3*H*-phenoxazin-3-one **E86**
N-(4-ethoxyphenyl)-acetamide **P58**
 4-ethoxy-7-phenyl-3,5-dioxa-6-aza-4-phosphaoct-6-ene-8-nitrile 4-sulfide **P170**
 4-ethoxyphenylurea **E81**
 1-ethoxypropane **E82**
 2-ethoxypropane **E83**
 1-ethoxy-2-propanol **E84**
 3-ethoxy-1-propene **A82**
 ethoxyquin **E85**
 7-ethoxyresorufin **E86**
 5-ethoxy-3-(trichloromethyl)-1,2,4-thiadiazole **E185**
 ethrane **E27**
 Ethrel **E63**
 Ethulose **F111**
 ethyl acetate **E87**
 ethylacetic acid **B285**
 ethyl acetoacetate **E88**
 ethylacetone **M292**
 ethyl acetyl acetate **E88**

ethylacetylene **B281**
 ethyl acrylate **E89**
 ethyl adipate **E136**
 ethyl adipate **D287**
 ethylal **D286**
 ethyl alcohol **E61**
 ethylaldehyde **A7**
 ethyl all-*trans*-9-(4-methoxy-2,3,6-trimethyl phenyl)-3,7-dimethylnona-2,4,6,8-tetraenoate **E184**
 ethyl allyl ether **A82**
 ethylamine **E90**
N-ethylaminobenzene **E95**
p-ethylaminobenzene **E94**
 ethyl *p*-aminobenzoate **B55**
 2-ethylamino-4-isopropylamino-6-methylmercapto-s-triazine **A109**
 2-(ethylamino)-4-(isopropylamino)-6-(methylthio)-s-triazine **A109**
 2-(ethylamino)-4-methyl-5-*n*-butyl-6-hydroxypyrimidine **E70**
 ethyl *p*-aminophenyl ketone **A149**
 ethyl ammonium (aminocarbonyl)phosphonate **F107**
 ethyl amyl ketone **E91**
 ethyl *n*-amyl ketone **E91**
 ethyl *sec*-amyl ketone **M230**
 ethylaniline **E95**
 2-ethylaniline **E92**
 3-ethylaniline **E93**
 4-ethylaniline **E94**
m-ethylaniline **E93**
N-ethylaniline **E95**
o-ethylaniline **E92**
p-ethylaniline **E94**
 2-ethyl-9,10-anthracenedione **E96**
 2-ethylanthraquinone **E96**
 β-ethylanthraquinone **E96**
 ethyl arsonous dichloride **E112**
 5-ethyl azepane-1-carbothioate **M337**
 2-ethylbenzenamine **E92**
 3-ethylbenzenamine **E93**
 4-ethylbenzenamine **E94**
N-ethylbenzenamine **E95**
 ethylbenzene **E97**
 4-ethyl-1,3-benzenediol **E98**
p-ethylbenzenediol **E98**
 ethyl benzoate **E99**
 2-ethyl-3-benzofuranyl-*p*-hydroxyphenyl ketone **B44**
 (2-ethyl-3-benzofuranyl)(4-hydroxyphenyl) methanone **B44**
 ethyl *O*-benzol-3-chloro-2,6-dimethoxybenzohydroximate **B81**
 ethyl *N*-benzoyl-*N*-(3,4-dichlorophenyl)-2-aminopropionate **B84**
 ethylbenzylaniline **E100**
N-ethyl-*N*-benzylaniline **E100**
 ethyl(*Z*)-*N*-benzyl-*N*-[[methyl(1-methylthioethylidene-amino-oxycarbonyl)amino]thio]-β-alaninate **A61**
 ethylbis(2-chloroethyl)amine **H82**
S-ethyl bis(2-methylpropyl)carbamothioate **B243**
O-ethyl *S,S*-bis(1-methylpropyl) phosphorodithioate **C15**
 ethyl borate **E101**
 ethyl bromide **B175**
 ethyl bromoacetate **E102**
 ethyl 2-bromoacetate **E102**
 ethyl bromoethanoate **E102**
 2-ethylbutanal **E104**
 ethyl butanoate **E105**
 2-ethylbutanol **E103**
 2-ethyl-1-butanol **E103**
 2-ethylbutan-1-ol **E103**
 2-ethyl-*n*-butanol **E103**
E-ethyl butenoate **E109**
 ethyl butex **E158**
 ethylbutylacetaldehyde **E125**
 2-ethylbutyl alcohol **E103**
 5-ethyl-5-*N*-butylbarbituric acid **B222**
 ethyl butyl ether **B257**
 ethyl butyl ketone **H24**
 2-ethylbutyraldehyde **E104**
 α-ethylbutyraldehyde **E104**
 ethyl butyrate **E105**
 ethyl *n*-butyrate **E105**
 2-ethylbutyric aldehyde **E104**
 α-ethylcaproaldehyde **E125**
 α-ethylcaproic acid **E127**
 ethyl carbamate **U13**
S-(*N*-ethylcarbamoylmethyl) *O,O*-dimethyl phosphorodithioate **E71**
 9-ethyl-9*H*-carbazol-3-amine **A128**
 ethylcarbinol **P296**
 ethyl δ-(carboethoxyvalerate) **D287**
 ethyl carbonate **D298**
 ethyl cellosolve **E76**
 ethyl cellosolve acetate **E79**
 ethyl centralite **D297**
 ethyl chloride **C196**
 ethyl chloroacetate **E106**
 ethyl α-chloroacetate **E106**
 (±)-ethyl 2-[4-[(6-chloro-2-benzoxazolyl)oxy]phenoxy]-propanoate **F16**
 ethyl chlorocarbonate **E107**
 ethyl chloroethanoate **E106**
 ethyl chloroformate **E107**
 ethyl chlorophenoxyisobutyrate **C358**
 ethyl α-(*p*-chlorophenoxy)isobutyrate **C358**
 ethyl 2-(4-chlorophenoxy)-2-methylpropionate **C358**
 ethyl 2-chloropropionate **E108**
 ethyl α-chloropropionate **E108**
 (±)-ethyl 2-chloropropionate **E108**
 ethyl citrate **T279**
 ethyl clofibrate **C358**
 ethyl crotonate **E109**
 (*E*)-ethyl crotonate **E109**
 ethyl *trans*-crotonate **E109**

N-ethyl-*o*-crotonotoluidide **C466**
 ethyl cyanide **P312**
 ethyl cyanoacetate **E110**
 ethyl 2-cyanoacetate **E110**
 ethyl cyanoethanoate **E110**
 ethylcyclohexane **E111**
 5-ethyl cyclohexyl(ethyl)thiocarbamate **C498**
 5-ethyl *N*-cyclohexyl-*N*-ethyl(thiocarbamate) **C498**
p,p'-ethyl DDD **D199**
 ethyldichloroarsine **E112**
 ethyl 4,4'-dichlorobenzilate **C164**
 ethyl *p,p*-dichlorobenzilate **C164**
 ethyl 2-[(diethoxyphosphinothioyl)oxy]-5-methylpyrazolo-[1,5-*a*]pyrimidine-6-carboxylate **P350**
 ethyl *N*-(diethoxythiophosphorylthio)acetyl-*N*-methylcarbamate **M37**
 ethyl 2-diethoxythiophosphoryloxy-5-methylpyrazolo[1,5-*a*]pyrimidine-6-carboxylate **P350**
 ethyl diglyme **E80**
 ethyl *N*-[2,3-dihydro-2,2-dimethylbenzofuran-7-yloxy carbonyl(methyl)aminothio]-*N*-isopropyl- β -alaninate **B30**
 (3*S*-*cis*)-3-ethyldihydro-4-[(1-methyl-1*H*-imidazol-5-yl)methyl]-2(3*H*)-furanone **P189**
 3-ethyldihydro-4-[(1-methyl-*H*-imidazol-5-yl)methyl]-2(3*H*)-furanone, monohydrochloride **P190**
 1-ethyl-1,4-dihydro-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid **N4**
 5-ethyldihydro-5-phenyl-4,6(1*H*,5*H*)-pyrimidinedione **P272**
 ethyl *N,N*-diisobutylthiocarbamate **B243**
 ethyl 2-dimethoxyphosphinothioyl(phenyl) acetate **P89**
 ethyl α -(dimethoxyphosphinothioyl)thio]benzeneacetate **P89**
N-ethyldimethylamine **D414**
 ethyldimethylcarbinol **M173**
 2-ethyl-1,1-dimethylethylene **M283**
 ethyldimethylmethane **M172**
 ethyldimethyl(1-methyl-3,3-diphenylpropyl) ammonium bromide **E16**
 (Z-ethyl 3,7-dimethyl-6-oxo-9-(phenylmethyl)-5-oxa-2,8-dithia-4,7,9-triazadodec-3-en-12-oate **A61**
 ethyl *N*-dimethylphosphoramidocyanidate **T2**
 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoic acid, 2-ethylhexyl ester **D521**
O-ethyl *S,S*-diphenyl phosphorodithioate **E2**
S-ethyl dipropylcarbamothioate **E40**
O-ethyl-*S,S*-dipropyl phosphorodithioate **E74**
 ethyl *N,N*-dipropylthiocarbamate **E40**
S-ethyl dipropylthiocarbamate **E40**
 ethylene **E113**
 ethylene aldehyde **A35**
 1,1'-ethylene-2,2'-bipyridyldiylum **D560**
 ethylene bis(dithiocarbamate), mixed metal complex containing $\leq 8.15\%$ (*m/m*) zinc, 8.05% (*m/m*) magnesium, 5.5% (*m/m*) copper and 1.0% (*m/m*) iron **C473**
 ethylene bis(dithiocarbamate)manganese **M21**
 ethylenebis(dithiocarbamate)zinc **Z18**
 ethylene carboxamide **A41**
 ethylenecarboxylic acid **A42**
 ethylene chloride **D211**
 ethylene chlorobromide **B170**
 ethylene chlorohydrin **C197**
 ethylene, chlorotris(*p*-methoxyphenyl)- **C299**
 ethylene cyanide **S130**
 ethylenediamine **E114**
 ethylenediamine, compound with theophylline **A147**
 ethylenediaminetetraacetate copper chelate **E5**
 ethylenediaminetetraacetic acid **E3**
 ethylenediaminetetraacetic acid, tetrasodium salt **E8**
N,N,N',N'-ethylenediaminetetramethylende phosphonic acid **E11**
 ethylenediaminetetramethylphosphonic acid **E11**
 ethylene dibromide **D132**
 1,2-ethylene dibromide **D132**
cis-1,2-ethylenedicarboxylic acid **M12**
trans-1,2-ethylenedicarboxylic acid **F115**
 ethylene dichloride **D211**
 ethylene dimercaptan **E59**
 ethylene dimethacrylate **E119**
 ethylene dimethyl ether **D381**
 ethylene dinitrate **E115**
 (ethylenedinitrilo)tetraacetic acid **E3**
 (ethylenedinitrilo)tetraacetic acid copper(II) complex **E5**
 (ethylenedinitrilo)tetraacetic acid tetrasodium salt **E8**
 (ethylenedinitrilo)tetraacetic acid, trisodium salt **E9**
 (ethylenedinitrilo)tetracetic acid, dipotassium salt **E6**
 2,2'-ethylenedioxydiethanol **T280**
 2,2'-(ethylenedioxy)diethyl diacrylate **T281**
 ethylene dithioglycol **E59**
 ethylenedithiol **E59**
 ethylene episulfide **E121**
 ethylene fluorohydrin **F65**
 ethylene glycol **E116**
 ethylene glycol acetate **E117**
 ethylene glycol bis(2,3-epoxypropyl) ether **E118**
 ethylene glycol, chlorohydrin **C197**
 ethylene glycol dibutyl ether **D138**
 ethylene glycol diethyl ether **D285**
 ethylene glycol diglycidyl ether **E118**
 ethylene glycol dimethacrylate **E119**
 ethylene glycol dimethyl ether **D381**
 ethylene glycol dinitrate **E115**
 ethylene glycol ethyl ether **E76**
 ethylene glycol homopolymer **P225**
 ethylene glycol isopropyl ether **I119**
 ethylene glycol monoacetate **E117**
 ethylene glycol monobutyl ether **B226**
 ethylene glycol monoethyl ether **E76**
 ethylene glycol monoethyl ether acetate **E79**
 ethylene glycol monomethyl ether **M134**
 ethylene glycol monomethyl ether acetate **M136**
 ethylene glycol monophenyl ether **P86**

ethylene glycol monopropyl ether **P316**
ethylene glycol mono-*n*-propyl ether **P316**
ethylene glycol monosalicylate **G38**
ethylene methacrylate **E119**
ethylene monochloride **V30**
1,8-ethylenenaphthalene **A3**
ethylene oxide **E120**
ethylene sulfide **E121**
ethylene tetrachloride **T51**
ethylenethiourea **E122**
N,N'-ethylenethiourea **E122**
ethylene trichloride **T249**
ethylenimine **A266**
ethyl ethanoate **E87**
ethyl ether **D304**
m-ethylethylbenzene **D293**
p-ethylethylbenzene **D294**
3-ethyl-2-[5-(3-ethyl-2-(3*H*)-benzothiazolylidene-1,3-pentadienyl)benzothiazolium iodide **D571**
ethylethylene **B215**
ethylethylene oxide **E36**
2-ethyl-*N*-(2-ethylhexyl)-1-hexanamine **D515**
N-ethyl-*N*-[4-[[4-[ethyl[(3-sulfophenyl)methyl]amino]-phenyl](4-hydroxy-2-sulfophenyl)-methylene]-2,5-cyclohexadien-1-ylidene]-3-sulfobenzene-methanaminium hydroxide inner salt, disodium salt **C412**
N-ethyl-*N*-(4-[[4-[ethyl[(3-sulfophenyl)methyl]amino]-phenyl]phenylmethylene]-2,5-cyclohexadien-1-ylidene)-3-sulfobenzenemethanaminium hydroxide, inner salt, sodium salt **C388**
ethylethyne **B281**
ethyl fluoride **F64**
ethyl formate **E123**
ethylformic acid **P310**
1-ethyl-1-formylhydrazine **E124**
N-ethyl-*N*-formylhydrazine **E124**
ethyl glycol acetate **E79**
O-ethylglycol acetate **E79**
ethyl guthion **A263**
N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-1-octanesulfonamide **S142**
ethyl heptazine **E73**
5-ethylhexahydro-4,6-dioxo-5-phenylpyrimidine **P272**
([2*S*-[2 α (*S**),3 β ,11 β]]-3-ethyl-1,3,4,6,7,11*b*-hexahydro-2-[(1,2,3,4-tetrahydro-1-isoquinoliny)methyl]-2*H*-benzo[*a*]quinolizine) dihydrochloride **E17**
2-ethylhexaldehyde **E125**
2-ethylhexanal **E125**
2-ethyl-1,3-hexanediol **E126**
2-ethylhexanoic acid **E127**
2-ethylhexanol **E128**
2-ethyl-1-hexanol **E128**
2-ethyl-1-hexanol hydrogen phosphate **D518**
2-ethyl-1-hexanol phosphate **T355**
2-ethylhexenal **E129**
2-ethyl-2-hexenal **E130**
2-ethylhexyl acrylate **E131**
(\pm)-2-ethylhexyl acrylate **E131**
2-ethylhexyl alcohol **E128**
2-ethylhexylamine **E132**
(\pm)-2-ethylhexylamine **E132**
2-ethylhexyl carbonochloridic acid **E133**
2-ethylhexyl chloroformate **E133**
(\pm)-2-ethylhexyl chloroformate **E133**
ethylhexylene glycol **E126**
2-ethylhexyl hydrogen phthalate **M344**
2-ethylhexyl mercaptoacetate **E134**
2-ethylhexylphenol **E135**
(2-ethylhexyl)phenol **E135**
2-ethylhexyl phthalate **D519**
2-ethylhexyl 2-propenoate **E131**
ethyl hydrate **E61**
ethyl hydride **E58**
ethyl hydrogen adipate **E136**
ethyl hydrogen hexanedioate **E136**
ethyl hydrogen sulfate **E173**
ethyl hydropersulfide **E59**
ethyl hydrosulfide **E60**
ethyl hydroxide **E61**
1-ethyl-2-hydroxybenzene **E160**
1-ethyl-4-hydroxybenzene **E162**
ethyl 2-hydroxybenzoate **E169**
ethyl 3-hydroxybenzoate **E137**
ethyl 4-hydroxybenzoate **E158**
ethyl *m*-hydroxybenzoate **E137**
ethyl *p*-hydroxybenzoate **E158**
2-ethyl-4'-hydroxy-3-benzoylbenzofuran **B44**
ethyl 2-hydroxy-2,2-bis(4-chlorophenyl)acetate **C164**
2-ethyl-2-(hydroxymethyl)-, cyclic phosphite **T310**
 α -ethyl- β -(hydroxymethyl)-1-methylimidazole-5-butyric acid, γ -lactone **P189**
2-ethyl-2-(hydroxymethyl)-1,3-propanediol triacrylate **T311**
ethyl 2-hydroxypropanoate **E141**
(*S*)-ethyl 2-hydroxypropanoate **E142**
ethyl 2-hydroxypropionate **E141**
ethyl α -hydroxypropionate **E141**
ethylic acid **A12**
Ethyl Icinol **E76**
ethylideneacetone **P44**
5-ethylidenebicyclo[2.2.1]hept-2-ene **E138**
ethylidene chloride **D210**
ethylidene dichloride **D210**
ethylidene diethyl ether **A6**
ethylidene dimethyl ether **D380**
ethylidene fluoride **D330**
ethylidene gyromitrin **A8**
trans-15-ethylidene-12 β -hydroxy-12 α -hydroxymethyl-13-methylenesene-1-ene **R14**
trans-15-ethylidene-12 β -hydroxy-4,12 α ,13 β -trimethyl-8-oxo-4,8-secosene-1-ene **S23**
ethylidene methyl hydrazine carboxaldehyde **A8**
ethylidenenorbornene **E138**

5-ethylidene-2-norbornene **E138**
 ethylidene hydroxylamine **A9**
 ethylimine **A266**
 ethyl iodide **I49**
 ethyl isoamyl ketone **M230**
 ethyl isobutanoate **E139**
 ethyl isobutyrate **E139**
 ethyl isocyanate **E140**
 5-ethyl-5-isopentylbarbituric acid **A204**
 ethyl isopropyl carbinol **M278**
 ethyl isopropyl ether **E83**
 (RS)-5-ethyl-2-(4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl)nicotinic acid **I7**
 ethyl ketone **D307**
 ethyl lactate **E141**
 L-ethyl lactate **E142**
 (-)-ethyl lactate **E142**
 S-(-)-ethyl lactate **E142**
 ethyl mercaptan **E60**
 ethylmercaptophenyl acetate (S)-ester with O,O-dimethylphosphorodithioacetate **P89**
 ethylmercuric chloride **E143**
 ethylmercuric phosphate **E144**
 ethylmercury **D308**
 ethylmercury(II) chloride **E143**
 ethylmercury(II) phosphate **E144**
 ethyl methacrylate **E145**
 ethyl methanesulfonate **E146**
 ethyl methanoate **E123**
 ethyl 2-methylacrylate **E145**
 ethyl α -methylacrylate **E145**
 N-ethyl-N-methylallyl-4-trifluoromethyl-2,6-dinitroaniline **E56**
 1-ethyl-2-methylbenzene **E176**
 1-ethyl-3-methylbenzene **E177**
 1-ethyl-4-methylbenzene **E178**
 ethyl 4-methylbenzenesulfonate **E179**
 5-ethyl-5-(1-methylbutyl)barbituric acid **P45**
 5-ethyl-5-(1-methylbutyl)-2,4,6-(1H,3H,5H)-pyrimidinetrione **P45**
 5-ethyl-5-(3-methylbutyl)-2,4,6-(1H,3H,5H)-pyrimidinetrione **A204**
 ethyl methylene phosphorodithioate **E68**
 ethyl methyl ether **E147**
 N-ethyl-N'-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine **A109**
 ethyl methyl ketone **M220**
 ethyl methyl ketoxime **M221**
 N-ethyl-2-methylmaleimide **E148**
 O-ethyl O-[4-(methylmercapto)phenyl] S-n-propyl phosphorothionothioate **S159**
 ethylmethylnitrosamine **N161**
 ethyl methylnitrosocarbamate **N164**
 2-ethyl-2-[[[(2-methyl-1-oxo-2-propenyl)oxy]methyl]-1,3-propanediyl **T312**
 N-ethyl-N-(2-methylphenyl)-2-butenamide **C466**
 N-ethyl-N-(2-methylphenyl)crotonamide **C466**
 ethyl methyl phosphorodithioate **D310**
 ethyl 2-methylpropanoate **E139**
 1-ethyl-1-methyl-1-propanol **M279**
 ethyl 2-methylpropenoate **E145**
 N-ethyl-N-(2-methyl-2-propenyl)-2,6-dinitro-4-(trifluoromethyl)benzenamine **E56**
 ethyl 2-methylpropionate **E139**
 2-ethyl-5-methylpyrazine **E149**
 5-ethyl-2-methylpyridine **E163**
 1-ethyl-3-methyl-1H-pyrrole-2,5-dione **E148**
 1-ethyl-3-methylpyrrole-2,5-dione **E148**
 O-ethyl O-[4-(methylthio)phenyl] methylphosphonothioate **E150**
 O-ethyl O-[4-(methylthio)phenyl]-phosphorodithioic acid S-propyl ester **S159**
 N-ethyl- α -methyl-3-(trifluoromethyl) phenylethylamine **F9**
 ethyl monochloroacetate **E106**
 ethyl monosulfide **E172**
 ethylmorphine **E151**
 3-O-ethylmorphine **E151**
 ethylmorpholine **E152**
 4-ethylmorpholine **E152**
 N-ethylmorpholine **E152**
 Ethyl Namate **D575**
 ethyl naphtha **G8**
 1-ethylnaphthalene **E153**
 2-ethylnaphthalene **E154**
 ethyl 1-naphthaleneacetate **E155**
 ethyl 1-naphthylacetate **E155**
 ethylnitrile **A20**
 ethyl nitrite **E156**
 O-ethyl O-(4-nitrophenyl) phosphonothioate **E35**
 O-ethyl O-(p-nitrophenyl) phosphonothioate **E35**
 ethyl p-nitrophenyl thionobenzenephosphonate **E35**
 ethylnitrosoaniline **N157**
 N-ethyl-N-nitrosobenzenamine **N157**
 ethylnitrosocyanamide **E157**
 N-ethyl-N-nitrosoethanamine **N149**
 1-ethyl-1-nitrosoarea **N158**
 1-ethyl-3-(5-nitro-2-thiazolyl)urea **N63**
 N-ethyl-N'-(5-nitro-2-thiazolyl)urea **N63**
 O-ethyl O-6-nitro-m-tolyl-sec-butyl phosphoramidothioate **B198**
 1-(β -ethylol)-2-methyl-5-nitro-3-azapyrrole **M327**
 ethyl orthoformate **T286**
 ethyl oxalate **D312**
 ethyloxirane **E36**
 ethyl 3-oxobutanoate **E88**
 2-ethyl-2-[[[(1-oxo-2-propenyl)oxy]methyl]-1,3-propanediyl propenoate **T311**
 ethylparaben **E158**
 ethyl paraben **E158**
 ethyl perchlorate **E159**
 N-ethylperfluoro-octane-1-sulfonamide **S142**
 S-ethyl perhydroazepine-1-carbothioate **M337**
 S-ethyl perhydroazepine-1-thiocarboxylate **M337**

2-ethylphenol **E160**
 3-ethylphenol **E161**
 4-ethylphenol **E162**
 o-ethylphenol **E160**
 p-ethylphenol **E162**
 ethyl 2-(4-phenoxyphenoxy)ethylcarbamate **F17**
 ethylphenylamine **E95**
 3-ethylphenylamine **E93**
 4-ethylphenylamine **E94**
 N-ethyl-N-phenylamine **E95**
 5-ethyl-5-phenylbarbituric acid **P79**
 N-ethyl-N-phenylbenzenemethanamine **E100**
 ethyl 3'-phenylcarbamoyloxycarbanilate **D59**
 ethyl 3-phenylcarbamoyloxyphenylcarbamate **D59**
 ethyl(phenyl)dichlorosilane **D215**
 3-ethyl-3-phenyl-2,6-dioxopiperidine **G22**
 ethyl phenyl ether **P73**
 O-ethyl S-phenyl ethyl phosphonothiolothionate **F99**
 2-ethyl-2-phenylglutarimide **G22**
 5-ethyl-5-phenyl-2,4,6-(1H,3H,5H)-pyrimidinetrione **P79**
 ethyl phosphate **T287**
 ethylphosphonodithioic acid O-ethyl S-phenyl ester **F99**
 ethyl phthalate **D314**
 5-ethyl-2-picoline **E163**
 1-ethylpiperidine **E164**
 N-ethylpiperidine **E164**
 2-ethylpropanal **M183**
 ethyl 2-propenoate **E89**
 ethyl propionate **E165**
 2-ethyl-3-propylacrolein **E130**
 α-ethyl-β-n-propylacrolein **E130**
 N-(1-ethylpropyl)-3,4-dimethyl-2,6-dinitrobenzenamine **P20**
 N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine **P20**
 ethyl propyl ether **E82**
 ethyl propyl ketone **H68**
 2-ethyl-3-propyl-1,3-propanediol **E126**
 ethyl PTS **E179**
 ethyl pyrazinyl phosphorothioate **T135**
 2-ethylpyridine **E166**
 3-ethylpyridine **E167**
 4-ethylpyridine **E168**
 γ-ethylpyridine **E168**
 2-ethyl-4-pyridinecarbothioamide **E69**
 4-ethylresorcinol **E98**
 6-ethylresorcinol **E98**
 ethyl rhodanate **E175**
 ethyl salicylate **E169**
 ethyl silicate **T67**
 ethylsilicon trichloride **E180**
 3-ethylstyrene **E170**
 4-ethylstyrene **E171**
 m-ethylstyrene **E170**
 p-ethylstyrene **E171**
 ethyl sulfate **D317**
 ethyl sulfhydrate **E60**
 ethyl sulfide **E172**
 S-[2-(ethylsulfinyl)ethyl] O,O-dimethyl phosphorothioate **O57**
 ethyl sulfocyanate **E175**
 S-[2-ethylsulfonyl]ethyl] O,O-dimethyl phosphorothioate **D55**
 1-[5-ethyl sulfonyl-1,3,4-thiadiazol-2-yl]-N,N'-dimethylurea **E64**
 ethylsulfuric acid **E173**
 ethyl tellurac **E174**
 ethyl tetraphosphate **H44**
 ethyl thioalcohol **E60**
 (N-(2-ethylthio)benzene sulfonamido-S,O,O-diisopropylphosphorodithioate **B36**
 2-(ethylthio)-4,6-bis(isopropylamino)-s-triazine **D551**
 6-(ethylthio)-N,N'-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine **D551**
 ethyl thiocyanate **E175**
 ethylthiodemeton **D566**
 ethylthioethane **E172**
 S-[2-(ethylthio)ethyl] O,O-dimethyl phosphorodithioate **T134**
 S-2-ethylthioethyl O,O-dimethyl phosphorodithioate **T134**
 [2-(ethylthio)ethyl] O,O-dimethylphosphorothioate **D50**
 O-2-ethylthioethyl O,O-dimethyl phosphorothioate **D52**
 O-[2-(ethylthio)ethyl] O,O-dimethyl phosphorothioate **D52**
 S-[2-(ethylthio)ethyl] O,O-dimethyl phosphorothioate **D54**
 S-2-ethylthioethyl O,O-dimethyl phosphorothioate **D54**
 2-ethylthioisonicotinamide **E69**
 2-[(ethylthio)methyl]phenol, methylcarbamate **E67**
 2-(ethylthio)methylphenyl N-methylcarbamate **E67**
 ethylthiometon sulfoxide **D567**
 ethyl thiophanate **T137**
 2-ethyltoluene **E176**
 3-ethyltoluene **E177**
 4-ethyltoluene **E178**
 m-ethyltoluene **E177**
 o-ethyltoluene **E176**
 p-ethyltoluene **E178**
 ethyl 4-toluenesulfonate **E179**
 ethyl p-toluenesulfonate **E179**
 ethyl p-tosylate **E179**
 ethyl 3-trichloromethyl-1,2,4-thiadiazol-5-yl ether **E185**
 O-ethyl O-(2,4,5-trichlorophenyl)ester
 ethylphosphonothioate **T253**
 ethyltrichlorosilane **E180**
 N-ethyl-N-α,α,α-trifluoro-N-(2-methylallyl)-2,6-dinitro-p-toluidine **E56**
 16-ethyl-1,16,19-trimethoxy-4-(methoxymethyl)aconitane-3,8,10,11,18-pentol 8-acetate 10-benzoate **A33**
 ethyl (2E,4E)-3,7,11-trimethyldodeca-2,4-dienoate **H106**
 ethyl (2E,4E)-3,7,11-trimethyl-2,4-dodecadienoate **H106**
 ethyl 3,7,11-trimethyldodeca-2,4-dienoate **H106**
 N-ethyl-N,N,α-trimethyl-γ-phenylbenzenepropanaminium bromide **E16**

Ethyl Tuads **D565**
 Ethyl Tuex **D565**
 ethyl urethane **U13**
 ethyl vinyl ether **E181**
 ethylzimate **Z9**
 ethylziram **Z9**
 ethyne **A26**
 ethyne calcium derivate **C24**
 ethyne, dichloro- **D177**
 1,1'-(1,2-ethynediyl)bisbenzene **D539**
 ethynodiol acetate-mestranol mixt **O41**
 ethynodiol diacetate **E182**
 ethynodiol diacetate mixed with mestranol **O41**
 ethynylcarbinol **P301**
 ethynyldimethylcarbinol **M182**
 17 α -ethynylestradiol 3-methyl ether **M92**
 ethynylestrenol **L67**
 17 α -ethynyl-17-hydroxy-5(10)-estren-3-one **N205**
 17 α -ethynyl-3-methoxy-1,3,5(10)-estratriene-17- β -ol **M92**
 ethynylnortestosterone **N204**
 17 α -ethynyl-19-nortestosterone **N204**
 ethynyloestradiol **E66**
 etidronic acid **E183**
 Etocarb **E67**
 Etoglucide **T282**
 Etrenol (mesylate) **H84**
 etretinate **E184**
 etridiazole **E185**
 etrimfos **E186**
 Etrofolan **I116**
 Etrolene **F8**
 ETU **E122**
 Eucalyptol **C343**
 eugenic acid **E187**
 eugenol **E187**
 eugenol methyl ether **M223**
 Eulan WA new **E188**
 Euparen M **T191**
 Euphyllin **A147**
 Euponol WAQ **S76**
 Eurax **C466**
 Euraxil **C466**
 europium **E189**
 Euscopol **H123**
 Evans Blue **E190**
 Evantin **P319**
 Evasprin **P140**
 Evastin **C68**
 EVE **E181**
 Event **I7**
 Evercyn **H100**
 Evicom **P235**
 evipal **H76**
 Evital **N206**
 EVITS **P156**
 Evronal **Q3**
 Evron Red BG **C398**
 Exact-S **D456**
 Exal **V21**
 Excalibur **C534**
 exhaust gas **C76**
 exluton **L67**
 exocorpol **P218**
 Exolit 385 **P158**
 Exomycol gel **P117**
 expansin **P16**
 Explosive D **A182**
 Express **M328**
 exsiccated alum **A105**
 Extar Forte **D512**
 Extrox **Z12**
 Extrusil **C43**
 Exxal 6 **H65**
 F-116 **H46**
 F-461 **O56**
 F238 **D593**
 FA **F127**
 FAA **F53**
 Factor II (vitamin) **C368**
 Factor S **B112**
 Falben **F97**
 Famophos **F1**
 Famosept **P117**
 famphur **F1**
 Fan **E19**
 Fan **E20**
 Fancol CH **C324**
 FANFT **N118**
 Fantom **C313**
 FAP **K11**
 Farinex **S110**
 Farmin 80 **S111**
 Fasciolin **H38**
 Fastac **C543**
 Fast Blue Base B **D95**
 Fast Blue DSC Base **D95**
 Fast Dark Blue Base R **T172**
 Fast Garnet GBC Base **C424**
 Fast Green FCF **C412**
 Fastogen Blue-5110 **P176**
 Fast Red A (pigment) **C416**
 Fast Red Base GL **M261**
 Fast Red Base RL **M259**
 Fast Scarlet G **M260**
 Fast Yellow GC Base **C154**
 neo-fat 14 **M362**
 Fatex EK80 **C126**
 Fat Yellow **M320**
 Favistan **M122**
 Fazor **M14**
 FC 21 **D216**
 FC 31 **C200**
 FD&C Blue No. 2 **I26**
 FD&C Green No. 3 **C412**

FD&C Red No. 1 **C414**
 FD&C Red No. 19 **R9**
 FD&C Red No. 2 **A108**
 FD&C Yellow No. 6 **C415**
 FDNB **D476**
 Felben **D538**
 Felin **P360**
 Felmane **F84**
 Felzodox **Z12**
 FEMA 2683 **M161**
 FEMA No.2415 **E88**
 FEMA No. 2422 **E99**
 FEMA No. 2428 **E139**
 FEMA No. 2458 **E169**
 FEMA No.2468 **I102**
 FEMA No. 2562 **H72**
 FEMA No. 3045 **T35**
 FEMA No. 3107 **V17**
 FEMA No. 3558 **T34**
 Femergin **E44**
 Fenab **C124**
 Fenac **C124**
 Fen-All **T10**
 Fenam **D536**
 fenaminosulf **F2**
 fenamiphos **F3**
 fenarimol **F4**
 Fenasip **F4**
 Fenatrol **C124**
 fenazaflor **F5**
 fenazaquin **F6**
 Fenbaz **F28**
 fenbutatin oxide **F7**
 fenchlorfos **F8**
 Fenesterin **P65**
 Fenestrin **P65**
 fenfluramine **F9**
 fenformin **P74**
 Fenfosphorin **D527**
 fenfuram **F10**
 fenfurame **F10**
 Fenidin **F27**
 Fenidina **P58**
 Fenidon **P76**
 Fenilphrenzone **F29**
 Fenion **F11**
 fenitrothion **F11**
 Fenmedipham **P78**
 fenobucarb **F12**
 Fenocap **D505**
 Fenolovo **F26**
 fenoprofen **F13**
 fenoprop **F14**
 Fenormone **F14**
 fenothiocarb **F15**
 fenoxaprop-ethyl **F16**
 fenoxycarb **F17**

fenpropanate **F18**
 fenpropathrin **F18**
 fenpropidin **F19**
 fenpropimorph **F20**
 fenpyroximate **F21**
 fenson **F22**
 fensulfothion **F23**
 fenthion **F24**
 Fenthion-methyl **F24**
 fentichlor **T121**
 fentin acetate **F25**
 fentin chloride **T340**
 fentin hydroxide **F26**
 fenuron **F27**
 fenvalerate **F28**
 fenvalerate α **E49**
 (S-S)-fenvalerate **E49**
 Fenyramidol **P140**
 Feosol **I76**
 feprazone **F29**
 ferbam **F30**
 ferimzone **F31**
 Fermate **F30**
 Fermatin **F26**
 fermentation amyl alcohol **M174**
 fermenticide liquid **S150**
 Fernex **P209**
 fero 66 **I68**
 Ferradow **F30**
 ferric chloride **I69**
 ferric dextran **I70**
 ferric dimethyldithiocarbamate **F30**
 ferric fluoride **I71**
 ferric nitrate **I73**
 ferric oxide **I74**
 α -ferric oxide **I74**
 ferric sesquioxide **I74**
 ferric sulfate **I77**
 ferric trichloride **I69**
 ferric trifluoride **I71**
 ferrihemic acid **H12**
 ferriprotoporphyrin basic **H12**
 ferrocene **F32**
 ferroglucin **I70**
 Ferrone **I72**
 Ferros **P208**
 ferrous ammonium sulfate **I67**
 ferrous chloride **I68**
 ferrous diammonium disulfate **I67**
 ferrous dichloride **I68**
 ferrous sulfate **I76**
 FertiloX **C39**
 Ferulon **F27**
 Fervin **A71**
 FES **Z1**
 Fetazine **E4**
 Ficam **B28**

Ficsan **H69**
 Fidis **P306**
 Filitox **M111**
 Filter agent, Celatom FW-14 **D97**
 Finale **G18**
 Final Pellets **D535**
 fipronil **F33**
 fire damp **M112**
 Fire gum G **G51**
 Firemaster BP-6 **P219**
 Firemaster FF-1 **P219**
 Firemaster T23P **T352**
 Fitostim **G14**
 Fixofruit **D257**
 6FK **H45**
 Flammex AP **T352**
 flamprop-M-isopropyl **F35**
 flamprop-methyl **F34**
 Flavaxin **R12**
 flavone **F36**
 Fleet-X **M90**
 Flex **F98**
 flexazone **P96**
 Flexchlor **C132**
 Flexilon **Z25**
 Fliefos **C128**
 flint **S29**
 flint **Q1**
 flocoumafen **F37**
 Floghene **O63**
 Flo-Mor **P8**
 Florasan **I4**
 Florel **E63**
 flores martis **I69**
 Floropryl **I106**
 flowers of antimony **A227**
 Floxacillin **F41**
 fluazifop-butyl **F38**
 fluazifop-P-butyl **F39**
 Flubalex **B29**
 Fluben **D326**
 flubenzimine **F40**
 flucloxacillin **F41**
 flucofuron **F42**
 flucythrinate **F43**
 Fludrocortisone **F63**
 Fludrone **F63**
 flue gas **C76**
 fluenetil **F44**
 Fluenyl **F44**
 flumetralin **F45**
 fluoboric acid **F46**
 Fluohydrocortisone **F63**
 fluometuron **F47**
 Fluon **P232**
 Fluorakil 100 **F53**
 Fluoral **S66**

fluoranthene **F48**
 fluorene **F49**
 9H-fluorene **F49**
 fluoren-9-one **F50**
 9-fluorenone **F50**
 9H-fluoren-9-one **F50**
 N-9H-fluoren-2-ylacetamide **A23**
 2-fluorenylacetamide **A23**
 N-2-fluorenylacetamide **A23**
 N-fluoren-2-ylacetohydroxamic acid **H109**
 N-2-fluorenylacetohydroxamic acid **H109**
 N-(9H-fluoren-2-yl)-N-hydroxyacetamide **H109**
 fluorescein **F51**
 fluorescein sodium **C399**
 Fluorescite **C399**
 fluorhydric acid **H101**
 fluorine **F52**
 fluorine monoxide **O61**
 fluorine oxide **O61**
 Fluorinert FC 43 **P55**
 Fluorinse **S66**
 Fluoristan **T161**
 fluorite **F80**
 fluoroacetamide **F53**
 2-fluoroacetamide **F53**
 4'-fluoroacetanilide **F54**
 fluoroacetic acid **F55**
 2-fluoroacetic acid **F55**
 4'-fluoro-4-acetylaminobiphenyl **F62**
 fluoroacetyl chloride **F56**
 2-fluoroacetyl chloride **F56**
 4'-fluoro-4-aminobiphenyl **F57**
 2-fluoroaniline **F58**
 3-fluoroaniline **F59**
 4-fluoroaniline **F60**
 m-fluoroaniline **F59**
 o-fluoroaniline **F58**
 p-fluoroaniline **F60**
 2-fluorobenzenamine **F58**
 3-fluorobenzenamine **F59**
 4-fluorobenzenamine **F60**
 fluorobenzene **F61**
 N-(4'-fluorobiphen-4-yl)acetamide **F62**
 N-(4'-fluoro-4-biphenyl)acetamide **F62**
 4'-fluoro-(1,1-biphenyl)-4-amine **F57**
 fluoroboric acid **F46**
 fluorocarbon 12 **D204**
 fluorochloridone **F87**
 fluorochloroform **F78**
 fluorochloromethane **C200**
 9 α -fluorocortisol **F63**
 fluorocortisone **F63**
 fluorodichloromethane **D216**
 N-(fluorodichloromethylthio)phthalimide **D217**
 1,2,4-fluorodinitrobenzene **D476**
 1-fluoro-2,4-dinitrobenzene **D476**
 fluoroethane **F64**

fluoroethanoic acid **F55**
 2-fluoroethanol **F65**
 β-fluoroethanol **F65**
 fluoroethene **V33**
 1-fluoroethene **V33**
 2-fluoroethyl[1,1'-biphenyl]-4-acetate **F44**
 2-fluoroethyl 4-biphenylacetate **F44**
 2-fluoroethyl biphenyl-4-yl acetate **F44**
 fluoroethylene **V33**
 fluoroflex **P232**
 fluoroform **T292**
 fluoroformyl fluoride **C80**
 fluoroglycofen-ethyl **F66**
 1-fluoro-2-methylbenzene **F76**
 1-fluoro-4-methylbenzene **F77**
 (fluoromethyl)oxirane **E34**
 fluoromethyl sulfone **M114**
 fluoromide **F67**
 Fluorophene **F72**
 2-fluorophenol **F68**
 3-fluorophenol **F69**
 4-fluorophenol **F70**
m-fluorophenol **F69**
o-fluorophenol **F68**
N-(4-fluorophenyl)acetamide **F54**
 (±)-α-(2-fluorophenyl)-α-(4-fluorophenyl)-1*H*-1,2,4-triazole-1-ethanol **F93**
 fluorophosphoric acid **F71**
 5-fluoro-2,4(1*H*,3*H*)pyrimidinedione **F79**
 fluorosalan **F72**
 fluorosilicate **F73**
 fluorosilicic acid **F74**
 fluorosulfonic acid **F75**
 fluorosulfuric acid **F75**
 fluorosulfuric acid, methyl ester **M224**
 5-fluoro-1-(tetrahydro-2-furanyl)-2,4(1*H*,3*H*)-pyrimidine-dione, 5-fluoro-1-(tetrahydro-2-furyl)uracil **F118**
 2-fluorotoluene **F76**
 4-fluorotoluene **F77**
o-fluorotoluene **F76**
p-fluorotoluene **F77**
 fluorotributylstannane **T215**
 fluorotrichloromethane **F78**
 (11β,16α)-9-fluoro-11,17,21-trihydroxy-16-methylpregna-1,4-diene-3,20-dione **D62**
 9-fluoro-11β,17,21-trihydroxy-16α-methylpregna-1,4-diene-3,20-dione **D62**
 (11β)-9-fluoro-11,17,21-trihydroxypregn-4-ene-3,20-dione **F63**
 9-fluoro-11β,17,21-trihydroxypregn-4-ene-3,20-dione **F63**
 fluorotriphenylstannane **T341**
 5-fluorouracil **F79**
 Fluorox **C37**
 4'-fluoroxenylamine **F57**
 fluorspar **F80**
 Fluothane **H4**
 fluotrimazole **F81**
 fluoxetine hydrochloride **F82**
 flupropanate-sodium **F83**
 Fluracil **F79**
 Flural **B29**
 flurazepam **F84**
 flurenol-butyl **F85**
 fluridone **F86**
 Fluroblastin **F79**
 flurochloridone **F87**
 fluroxypyr **F88**
 flurprimidol **F89**
 flusilazol **F90**
 flusilazole **F90**
 flusulfamide **F91**
 flutolanil **F92**
 Flutriafe **F93**
 flutriafol **F93**
 fluvalinate **F94**
 τ-fluvalinate **F94**
 flux-calcined diatomaceous earth **D97**
 flux maag **N54**
 fluxofenim **F95**
 Flypel **D319**
 FNT **N59**
 FOE 1976 **M41**
 Folbex VA **B187**
 Folex **M89**
 Folgorat **B150**
 folic acid **F96**
 Folicet **F96**
 Folidol **P13**
 Folidol M **P14**
 Folimat **O32**
 follicular hormone **E53**
 follicular hormone hydrate **O25**
 folliculin **E53**
 folpet **F97**
 Foltaf **C58**
 Folvite **F96**
 fomesafen **F98**
 Fonganil **F119**
 Fongarid **F119**
 fonofos **F99**
 Food Green 1 **C388**
 Food Red 102 **C394**
 Food Red 103 **E29**
 Food Red 106 **C396**
 Food Red 105, sodium salt **R16**
 Food Violet 2 **B101**
 Forane **I105**
 Forate **P145**
 Forbel **F20**
 Foresite **O44**
 Forgoren **P365**
 formal **D382**
 formaldehyde **F100**
 formaldehyde bis(β-chloroethyl)acetal **B118**

formaldehyde cyanohydrin **G37**
 formaldehyde diethyl acetal **D286**
 formaldehyde dimethyl acetal **D382**
 formamide **F101**
 formamine **H57**
 Formetanat **F102**
 formetanate **F102**
 formetanate hydrochloride **F103**
 formic acid **F104**
 formic acid, allyl ester **A83**
 formic acid, butyl ester **B258**
 formic acid, cadmium salt **C9**
 formic acid, chloro-, allyl ester **A79**
 formic acid, cobalt(II) salt **C373**
 formic acid, isobutyl ester **I90**
 formic acid, isopropyl ester **I126**
 formic acid, methyl ester **M226**
 formic acid, 1-methylethyl ester **I126**
 formic acid, methylhydrazide **M227**
 formic acid, 2-methylpropyl ester **I90**
 formic acid, 2-propenyl ester **A83**
 formic acid, propyl ester **P331**
 formic anammonide **H100**
 formic 2-[4-(5-nitrofuryl)-2-thiazolyl] hydrazide **N59**
 formomalenic thallium **T105**
 formonitrile **H100**
 formothion **F105**
 formparanate **F106**
 2-(formylamino)-4-(5-nitro-2-furyl)thiazole **N118**
 2-formylbutane **M183**
 4-formylcyclohexene **T71**
 2-formyl-3,4-dihydro-2H-pyran **A36**
 N-formyldimethylamine **D416**
 p-formyldimethylaniline **D387**
 2-(2-formylhydrazino)-4-(5-nitro-2-furyl)thiazole **N59**
 formylic acid **F104**
 1-formyl-1-methylhydrazine **M227**
 1-formylnaphthalene **N7**
 2-formylnaphthalene **N8**
 β-formylnaphthalene **N8**
 formyloxirane **G27**
 2-formylpentane **M316**
 2-formylphenol **S4**
 formyl trichloride **C201**
 1-formyl-3,5,6-trimethyl-3-cyclohexene **I100**
 Foron **P147**
 Forquat **P11**
 Forron **T1**
 Forstgranulat **H69**
 Fortalgesic **P42**
 fortified HCH **H9**
 Fortral **P42**
 fosamine-ammonium **F107**
 Fosbrom **N3**
 Foschlor **T225**
 fosetyl-aluminium **F108**
 Fos-Fall "A" **T209**
 Fostex P **E183**
 fosthietan **F109**
 Fostion **P342**
 Fototar **C366**
 Fouramine brown AP **P363**
 Fouramine STD **T174**
 Fournine 85 **P363**
 Fournine D **P103**
 Fowler's solution **P239**
 FR 28 **S96**
 Framyetin **N36**
 francium **F110**
 Franklin Fibre **C44**
 Franocide **D295**
 Franozan **D295**
 Freemans white lead **L30**
 French chalk **T3**
 French Green **C431**
 Frenock **F83**
 Freon 113 **T269**
 Freon 116 **H46**
 Freon 12 **D204**
 Freon 152 **D331**
 Freon 21 **D216**
 Freon 218 **O7**
 Freon 23 **T292**
 Freon 31 **C200**
 Freon 12B2 **D131**
 Freon MF **F78**
 Freon TF **T269**
 Frieste flowers **P354**
 Frigen 113 **T269**
 Frigen 12 **D204**
 Frostan **Q11**
 β-D-fructofuranosyl α-D-glucopyranoside **S131**
 fructoline **L57**
 fructosan **F111**
 β-D-fructose **F111**
 D-fructose **F111**
 Fructyben **G14**
 Fruitdo **O50**
 Fruitguard AB **B240**
 Fruitguard DPA **D540**
 Fruitofix **N22**
 fruit sugar **F111**
 Frumin AL **D566**
 frusemide **F112**
 Fruttistore **D540**
 FT207 **F118**
 fthalide **P174**
 fuberidazole **F113**
 Fubotran **D260**
 p-fuchsin **C402**
 Fuchsine **M1**
 D-fucose **F114**
 Fuji-one **I132**
 Fulcin **G46**

Ful-Glo **C399**
 fulminic acid, mercury(II) salt **M73**
 fumaric acid **F115**
 fumaric acid, dichloride **F117**
 fumaric acid, iron (2+) salt (1:1) **I72**
 fumarin **F116**
 (fumaroyldioxy)bis[tributyltin] **T216**
 fumaryl chloride **F117**
 Fumesin **E72**
 Fundazol **B32**
 Fungaflor **I4**
 Fungazil **I4**
 Fungicidin **N210**
 Fungiclor **D260**
 Fungilon D **D594**
 Funginex **T295**
 Fungizir **Z19**
 Fungo **T138**
 Furacarb **C68**
 Furacin **N116**
 Furacon **B30**
 Furadantin **N115**
 furafluor **F118**
 Furalan **N115**
 furalaxyl **F119**
 2-furaldehyde **F120**
 3-furaldehyde **F121**
 furaltadone **F122**
 L-furaltadone hydrochloride **O49**
 furan **F123**
 2-furanacrolein **F131**
 2-furancarboxaldehyde **F120**
 2-furancarboxaldehyde **F120**
 3-furancarboxaldehyde **F121**
 2-furancarboxaldehyde, 5-nitro-, semicarbazone **N116**
 2,5-furandione **M13**
 2-furanemethanol **F127**
 N'-(2'-furanidyl)-5-fluorouracil **F118**
 2-furanmethanamine **F128**
 6,7-furanocoumarin **P344**
 2(5H)-furanone **F124**
 2,(3H)-furanone, dihydro- **B288**
 Furanthril **F112**
 2-(2-furanyl)-1H-benzimidazole **F113**
 4-(2-furanyl)-3-buten-2-one **F129**
 3-(2-furanyl)-2-propenal **F131**
 furathiazole **N117**
 furathiocarb **F125**
 Furatone **D350**
 furazolidone **F126**
 Furazone **N116**
 Furdan **C68**
 furfural **F120**
 3-furfural **F121**
 furfural acetone **F129**
 furfuran **F123**
 N-furfuryladenine **K11**
 furfuryl alcohol **F127**
 furfurylamine **F128**
 2-furfurylamine **F128**
 6-(furfurylamino)purine **K11**
 furfurylideneacetone **F129**
 2-furfurylidene acetone **F129**
 furidiazine **A137**
 Furloe **C312**
 furmecyclox **F130**
 Furmetamide **F130**
 Furmethanol **F122**
 furmethonol **O49**
 furnace black **C73**
 7H-furo[3,2-g][1]benzopyran-7-one **P344**
 furo[2',3:7,6]coumarin **P344**
 furo[4',5':6,7]coumarin **P344**
 furole **F120**
 Furore **F16**
 Furosemide **F112**
 Furoxone **F126**
 3-(1-furyl-3-acetyloethyl)-4-hydroxycoumarin **F116**
 3-(2-furyl)acrolein **F131**
 β-furylacrolein **F131**
 β-(2-furyl)acrolein **F131**
 furyl alcohol **F127**
 furylamide **F132**
 2-(2'-furyl)benzimidazole **F113**
 2-furylcarbinol **F127**
 furylfuramide **F132**
 α-2-furyl-5-nitro-2-furanacrylamide **F132**
 2-(2-furyl)-3-(5-nitro-2-furyl)acrylamide **F132**
 3-(α-furyl)propenal **F131**
 Furzoline **F122**
 Fusarex **T14**
 fusarium toxin **Z1**
 fused borax **S96**
 fused silica **S29**
 Fusilade **F39**
 Fusilade **F38**
 Fusko **C541**
 Fussol **F53**
 FW925 **N112**
 Fyrol DMMP **D430**
 Fyrol FR-2 **T353**
 Fyrol HB32 **T352**
 G 19258 **D370**
 G 315 **O44**
 G 570 **P143**
 GA **T2**
 gadolinium **G1**
 Gafamide CDD-518 **C381**
 Gainex **P143**
 galactasol **G51**
 D-galactomethylose **F114**
 Galation **F11**
 galaxolide **G2**
 Galben Tairel **B26**

Galcodine **C383**
 Gallant **H5**
 gallic acid bismuth basic salt **B131**
 gallic acid, propyl ester **P332**
 gallium **G3**
 gallium arsenide **G4**
 gallium(III) chloride **G7**
 gallium metal, liquid **G3**
 gallium metal, solid **G3**
 gallium nitrate **G5**
 gallium(III) nitrate **G5**
 gallium oxide **G6**
 gallium(III) oxide **G6**
 gallium sesquioxide **G6**
 gallium trichloride **G7**
 gallotannic acid **T6**
 Galokson **P11**
 Gamma W8 **C502**
 Gamophene **H41**
 Gandural **N209**
 Gantanol **S136**
 Gantrosan **S141**
 Gardcide **T60**
 Gardona **T60**
 Garosorb **C37**
 Garrot **C68**
 gasohol **G8**
 gasoline, natural **G8**
 Gastracid **P62**
 Gatch **P7**
 Gaucho **I8**
 Gauntlet **N209**
 Gazette **C83**
 GC 1106 **H32**
 GC 2996 **M351**
 GC 6506 **M311**
 GC 7887 **H45**
 GC 8993 **T340**
 Gebutox **D510**
 Gedex **P231**
 Geigy 19258 **D370**
 Geigy Blue 536 **E190**
 Gelamite D **G26**
 Gelcarin **C91**
 Gell II **S66**
 Gelloid **C91**
 Gelodan **C91**
 Gelva **P233**
 Gencor **H106**
 Genep **E40**
 Genesis **T128**
 Genetron 113 **T269**
 Genetron 12 **D204**
 Genetron 13 **C302**
 Genetron 21 **D216**
 Genetron 218 **O7**
 Genetron 22 **C192**
 Genicide **X3**
 genistein **G9**
 genisteol **G9**
 genisterin **G9**
 Genitron **A269**
 Genomol P **T350**
 Genoxal **C529**
 gentiopicroin **G10**
 gentiopicroside **G10**
 Gentrol **H106**
 Geodan **C140**
 Geofos **F109**
 geon **P222**
 Geonter **T20**
 geosmin **G11**
 Gepiron **M355**
 geranial **C351**
 geranialdehyde **C351**
 geraniol **G12**
 (*E*)-geraniol **G12**
 geranium crystals **D544**
 germane **G13**
 germanium hydride **G13**
 germanium tetrahydride **G13**
 Gerontine **S107**
 Gesafloc **T275**
 Gesamil **P302**
 Gesapax **A109**
 Gestageno **H115**
 Gettysolve-B **H60**
 Gettysolve-C **H20**
 G-M-F **B75**
 gibberellic acid **G14**
 (+)-gibberellic acid **G14**
 gibberellin A3 **G14**
 Gibefol **G14**
 Gibrel **G14**
 Giltex **S69**
 glacial acetic acid **A12**
 D-glaucine **G15**
 Glaucon **A51**
 Glean **C315**
 Glu-P-1 **G19**
 Glu-P-2 **G20**
 D-glucitol **S104**
 α -D-glucochloralose **C109**
 Glucodigin **D335**
 Glucophage **M100**
 α -D-glucopyranose **G16**
 D-glucopyranose, 2-([2-chloroethyl]nitrosoamino)-
 carbonyl]amino)-2-deoxy-, 1-(2-chloroethyl)-1-nitroso-3-
 (D-glucos-2-yl)urea **C307**
 D-glucopyranose, 2-deoxy-2-(3-methyl-3-nitrosoureido)-
S120
 β -D-glucopyranose, 4-O- β -D-galactopyranosyl **L3**
 β -D-glucopyranosiduronic acid, *p*-(α , β -diethyl-*p*-
 hydroxystyryl)phenyl, (*E*)- **S118**

β -D-glucopyranosiduronic acid, 4-[1-ethyl-2-(4-hydroxyphenyl)-1-butenyl]phenyl, (*E*)- **S118**
 7- β -D-glucopyranosyl-9,10-dihydro-3,5,6,8-tetrahydroxy-1-methyl-9,10-dioxo-2-anthracenecarboxylic acid **C86**
 (*R*)-10- β -D-glucopyranosyl-1,8-dihydroxy-3-(hydroxymethyl)-9(10*H*)-anthracenone **B3**
 (D-glucopyranosylthio)gold **A255**
 α -glucose **G16**
 α -D-glucose **G16**
 D-glucose **G17**
 5- β -D-glucoside **B107**
 β -D-glucosyloxymethylazoxymethane **C494**
 (1-D-glucosylthio)gold **A255**
 glufofinate-ammonium **G18**
 L-glutamic acid, 5-[2-[4-(hydroxymethyl)phenyl]hydrazide] **A59**
 β -N-[γ -L-(+)-glutamyl]-4-hydroxymethylphenylhydrazine **A59**
 glutaral **G21**
 glutaraldehyde **G21**
 glutaric dialdehyde **G21**
 glutethimide **G22**
 glyceraldehyde **G23**
 D-glyceraldehyde **G24**
 DL-glyceraldehyde **G23**
 (\pm)-glyceraldehyde **G23**
 (*R*)-(+)-glyceraldehyde **G24**
 DL-glyceric aldehyde **G23**
 glycerin **G25**
 glycerin dichlorohydrin **D219**
 glycerin epichlorohydrin **C265**
 glycerin guaiaacolate **G47**
 glycerin triacetate **T196**
 glycerin tricaprilate **T224**
 glycerite **T6**
 glycerol **G25**
 glycerol acetone **S101**
 glycerol dichlorohydrin **D219**
 glycerol dimethylketal **S101**
 glycerol ester hydrolase **L51**
 glycerol α -(2-methoxyphenyl) ether **G47**
 glycerol triacetate **T196**
 glycerol trichlorohydrin **T264**
 glycerol trinitrate **G26**
 glycerol tris(chloromethyl) ether **T351**
 glyceryl chloride **C265**
 glyceryl α -chlorohydrin **C265**
 glycerylguaiaacolate carbamate **M125**
 glyceryl guaiafate **G47**
 glyceryl triacetate **T196**
 glyceryl tributyrates **T223**
 glycidal **G27**
 glycidaldehyde **G27**
 glycidol **G28**
 glycidol oleate **G34**
 glycidyl acrylate **G29**
 glycidyl alcohol **G28**

glycidyl aldehyde **G27**
 glycidyl butyl ether **B259**
 glycidyl-*tert*-butyl-ether **B260**
 glycidyl ether **D337**
 glycidyl isopropyl ether **G30**
 glycidyl methacrylate **G31**
 glycidyl α -methylacrylate **G31**
 glycidyl methyl ether **G32**
 (\pm)-glycidyl methyl ether **G32**
 glycidyl methylphenyl ether **C460**
 glycidyl 2-methylphenyl ether **C461**
 glycidyl 4-nitrophenyl ether **G33**
 glycidyl octadecenoate **G34**
 glycidyl oleate **G34**
 glycidyl phenyl ether **G35**
 glycidyl propenates **G29**
 glycidyl *o*-tolyl ether **C461**
 glycine **G36**
 glycol alcohol **E116**
 glycol bis(hydroxyethyl) ester **T280**
 glycol chlorohydrin **C197**
 glycol dibromide **D132**
 glycol dibutyl ether **D138**
 glycol dichloride **D211**
 glycol 1,3-dichlorohydrin **D247**
 glycol diethyl ether **D285**
 glycol diglycidyl ether **E118**
 glycol dimethyl ether **D381**
 glycol dinitrate **E115**
 glycol methylene ether **D532**
 glycol methyl ether **M134**
 glycol monoacetate **E117**
 glycol monobutyl ether **B226**
 glycol monobutyl ether acetate **B229**
 glycol monochlorohydrin **C197**
 glycol monoethyl ether **E76**
 glycolonitrile **G37**
 glycol salicylate **G38**
 Glycomul LC **S103**
 glyconitrile **G37**
 Glycosperse 0-20 **P230**
 Glycosperse P20 **P228**
 Glycosthene **G36**
 Glycotuss **G47**
 Glydant **D446**
 glyme **D381**
 glyocoll **G36**
 glyoxal **G39**
 glyoxaldehyde **G39**
 Glyoxaline **I9**
 Glypesin **H75**
 Glyphen **P74**
 glyphosate **G40**
 glyphosine **G41**
 Glyrol **G25**
 Glysal **G38**
 Glysantin **E116**

Goal **O59**
 Gohsenol **P234**
 gold **G42**
 gold bronze **C429**
 gold chloride **G43**
 gold(III) chloride **G43**
 Gold Crest **C118**
 Goldenon **C59**
 Golden salt **S42**
 gold thioglucose **A255**
 gold trichloride **G43**
 goodrite **P222**
 Good-rite GP-223 **D513**
 Gophacide **P148**
 Gopha-Rid **Z14**
 Graincoat **C314**
 gramine **G44**
 Graminon **I133**
 Gramox **D560**
 Granamide **C319**
 Granosan **E143**
 Granosan M **E144**
 Granstar **M328**
 granulated sugar **S131**
 Granurex **N32**
 Granutox **P145**
 graphite **G45**
 Graphtol Blue BL **P176**
 Grapil **E186**
 Grapple **F39**
 Grasal Brilliant Yellow **M320**
 Grasex **C108**
 Graslan **T13**
 Gratibain **O40**
 Gravidox **P359**
 Grazon **P182**
 greenland spar **C472**
 green nickel oxide **N47**
 greenockite **C14**
 Green S **C389**
 green vitriol **I76**
 Grenade **C534**
 grey arsenic **A240**
 Grill 8 **P229**
 Grimacit **D260**
 griseofulvin **G46**
 (+)-griseofulvin **G46**
 grisofulvin **G46**
 Gropper **M328**
 Grotan **H51**
 Grouctide 75 **C286**
p-guaiacol **M144**
 guaiacol glyceryl ether carbamate **M125**
 Guaiacuran **G47**
 guaiphenesin **G47**
 guanidine hydrochloride **G48**
 guanidine monohydrochloride **G48**
 guanidine mononitrate **G49**
 guanidine nitrate **G49**
 guanidinium nitrate **G49**
 Guanidol **D594**
 guanine **G50**
 Guardian **F43**
 Guar Gum **G51**
 guazatine acetates **G52**
 gum **P222**
 Gum Arabic **G53**
 Gum cyamopsis **G51**
 gum ovaline **G53**
 gum Senegal **G53**
 gum turpentine oil **T374**
 gun-cotton **C98**
 Gunner **F35**
 gur flour **G51**
 Gusathion **A264**
 Gyne-merfen **P120**
ortho-gynol **O20**
 gynovlar **N207**
 gypsum **C45**
 gyromitrin **A8**
 H-69 **X4**
 $^2\text{H}_2$ **D61**
 Hache Uno Super **F38**
 haematoporphyrin IX **H13**
 haematoxylin **H14**
 hafnium **H1**
 hafnium chloride **H2**
 hafnium dicyclopentadiene dichloride **H3**
 hafnium tetrachloride **H2**
 hafnocene dichloride **H3**
 Haipen **C58**
 Haitin **F26**
 half-Myleran **E146**
 Hall Tress DIBA **D351**
 Halmark **E49**
 Halodorm **M119**
 Halokon **F38**
 Halon 1001 **B178**
 Halon 11 **F78**
 Halon 1202 **D131**
 halothane **H4**
 Halowax **H39**
 haloxyfop-ethoxyethyl **H5**
 haloxyfop-etotyl **H5**
 HALSO 99 **C288**
 Hamidop **M111**
 Hammer **I7**
 Hamp-ene 100 **E8**
 Hansa red G **C416**
 Haoc **B150**
 hard paraffin **P7**
 Harman **H6**
 harmane **H6**
 harmine **H7**

Harvade **D374**
 Harvest **G18**
 HBF 386 **A45**
 HCB **H33**
 HCBD **H34**
 HC Blue No. 2 **H8**
 HCCH **H9**
 HCDD mixture 1,2,3,7,8,9 isomer **H37**
 HCE **H16**
 HCF3 31 **C200**
 HCFC 21 **D216**
 HCH **H9**
 ε-HCH **L48**
 γ-HCH **H10**
 HCP **H41**
 HDPE **P224**
 heavy hydrogen **D61**
 heavy oil **C453**
 Hedeltra **P269**
 Helianthine **M271**
 Helio Fast Blue-BRN **P176**
 heliotropin acetal **P207**
 helium **H11**
 Hellacap **E74**
 Heloxy 61 **B259**
 hematin **H12**
 hematoporphyrin **H13**
 hematoxiline **H14**
 hematoxylin **H14**
 hemimellitene **T306**
 3,4,5-hemimellitenol **T323**
 Hemineurin **C360**
 hemometine **E17**
 Hempa **H58**
 hendecanal **U1**
 hendecanaldehyde **U1**
 hendecane **U2**
 hendecanoic acid **U4**
 hendecyl alcohol **U5**
 HENU **H111**
 HEOD **D276**
 heptachlor **H15**
 heptachlor epoxide **H16**
 3,4,5,6,7,8,8a-heptachlorodicyclopentadiene **H15**
 heptachloro-2,2-dimethyl-3-methylenenorborane
P221
 1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3a,4,7,7a-tetrahydro-4,7-
 methanoindan **H16**
 2,3,4,5,6,7,7-heptachloro-1a,1b,5,5a,6,6a-hexahydro-2,5-
 metheno-2*H*-indeno[1,2-*b*]oxirene **H16**
 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-4,7-methano-
 1*H*-indene **H15**
 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-4,7-*endo*-
 methanoindene **H15**
 heptacosafuorotributylamine **P55**
 1-heptadecanecarboxylic acid **S112**
 2-heptadecyl-2-imidazoline-1-ethanol **H17**
 1,6-heptadiene-3,5-dione, 1,7-bis(4-hydroxy-3-
 methoxyphenyl)- **C478**
 heptafluorobutanoic acid anhydride **H18**
 heptafluorobutyric anhydride **H18**
 heptaldehyde **H19**
 heptanal **H19**
 heptane **H20**
n-heptane **H20**
 1-heptanecarboxylic acid **O12**
 1-heptanethiol **H21**
 heptanoic acid **H22**
n-heptanoic acid **H22**
 heptan-2-one **H23**
 heptan-3-one **H24**
 2-heptanone **H23**
 3-heptanone **H24**
 4-heptanone **H25**
 1-heptene **H26**
cis-2-heptene **H27**
cis-3-heptene **H28**
n-heptene **H26**
 (Z)-2-heptene **H27**
 (Z)-3-heptene **H28**
 heptenophos **H29**
 hepthlic acid **H22**
 heptylacetylene **N200**
 heptyl carbinol **O13**
 heptylene **H26**
 heptyl hydride **H20**
n-heptylic acid **H22**
 heptyl mercaptan **H21**
 heptyl phthalate **D340**
 Hepzide **N63**
 Herald **F18**
 Herbadox **P20**
 Herbit **M33**
 Herbius **M323**
 Herbivit **M32**
 Herbogil **D512**
 Herboxone **P11**
 Hercul 2 **G26**
 Hercules AC528 **D531**
 Hercules AS **C98**
 Herlin **L50**
 Hermat Zn-MBT **Z10**
 herniarin **M133**
 Hero **E63**
 Herplex **I48**
 Herpron **I133**
 hesperidin **H30**
 hesperidine **H30**
 hesperidoside **H30**
 hesperitin-7-rhamnoglucoside **H30**
 HET **H44**
 Het Acid **C122**
 heteroauxin **I32**
 Hetoxide MPC **C456**

HETP **H44**
 hexabarbital **H76**
 Hexa-Betalin **P359**
 hexabis(β,β -dimethylphenethyl)distanthoxane **F7**
 hexabromobiphenyl **P219**
 2,2',4,4',5,5'-hexabromobiphenyl **H31**
 2,2',4,4',5,5'-hexabromo-1,1'-biphenyl **H31**
 2,4,5,2',4',5'-hexabromobiphenyl **H31**
 hexabutyldistanthianine **T222**
 1,1,1,3,3,3-hexabutyldistanthianine **T222**
 hexabutyldistanthoxane **T219**
 hexachlor **H9**
 hexachloroacetone **H32**
 2',3,4,4',5,6-hexachloro-2-aminodiphenyl ether and their respective *N*-methylsulfone derivatives **E188**
 hexachlorobenzene **H33**
 1,2,3,4,7,7'-hexachlorobicyclo[2.2.1]hepta-2,5-diene **H40**
 1,4,5,6,7,7-hexachlorobicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid **C122**
 1,4,5,6,7,7-hexachlorobicyclo[2.2.1]hept-5-enedicarboxylic anhydride **C123**
 hexachlorobutadiene **H34**
 hexachloro-1,3-butadiene **H34**
 1,1,2,3,4,4-hexachloro-1,3-butadiene **H34**
 hexachlorocyclohexane **H9**
 (1 α ,2 α ,3 α ,4 β ,5 β ,6 β)-1,2,3,4,5,6-hexachlorocyclohexane **L48**
 1 α ,2 α ,3 β ,4 α ,5 α ,6 β -hexachlorocyclohexane **H10**
 ϵ -hexachlorocyclohexane **L48**
 ϵ -1,2,3,4,5,6-hexachlorocyclohexane **L48**
 1,2,3,4,5,6-hexachlorocyclohexane, technical mixture of isomers **H9**
 hexachlorocyclopentadiene **H35**
 1,2,3,4,5,5-hexachloro-1,3-cyclopentadiene **H35**
 hexachlorocyclopentadiene dimer **M334**
 2,2a,3,3,4,7-hexachlorodecahydro-(1 α ,2 β ,2a β ,4 β ,4a β ,5 β ,6a β ,6b β ,7R)-1,2,4-methenocyclopenta[*cd*]pentalene-5-carboxaldehyde **E26**
 1,2,3,6,7,8-hexachlorodibenzodioxin **H36**
 1,2,3,6,7,8-hexachlorodibenzo-*p*-dioxin **H36**
 1,2,3,7,8,9-hexachlorodibenzo-*p*-dioxin **H37**
 1,2,3,7,8,9-hexachlorodibenzo[*b,e*][1,4]dioxin **H37**
 1,1,2,3,3a,7a-hexachloro-5,6-epoxydecahydro-2,4,7-methano-1*H*-cyclopenta[*a*]pentalene, stereoisomer **P168**
 hexachloroepoxyoctahydro-*endo,endo*-dimethanonaphthalene **E25**
 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-*endo,endo*-1,4:5,8-dimethanonaphthalene **E25**
 hexachloroethane **H38**
 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4,5,8-*endo,endo*-dimethanonaphthalene **I101**
 1,2,3,4,10,10-hexachloro-1 α ,4 α ,4a β ,5 α ,8 α ,8a β -hexahydro-1,4:5,8-dimethanonaphthalene **A65**
 (1R,4S,4aS,5S,8R,8aR)-1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4:5,8-dimethanonaphthalene **A65**
 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-*exo*-1,4-*endo*-5,8-dimethanonaphthalene **A65**
 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3-benzodioxathiepin-3-oxide **E19**
 3,3',4,4',6,6'-hexachloro-2,2'-methylenediphenol **H41**
 hexachloronaphthalene **H39**
 1,2,3,4,7,7'-hexachloronorborene **H40**
 1,4,5,6,7,7-hexachloro-5-norborene-2,3-dicarboxylic acid **C122**
 1,4,5,6,7,7-hexachloro-5-norborene-2,3-dimethanal cyclic sulfate **E21**
exo-1,4,5,6,7,7-hexachloro-5-norborene-2,3-dimethanol **E20**
 1,4,5,6,7,7-hexachloro-5-norborene-2,3-dimethanol cyclic sulfite **E19**
 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-2,7:3,6-dimethanonaphth[2,3-*b*]oxirene **D276**
 1,2,3,4,10,10-hexachloro-1R,4S,4aS,5R,6R,7S,8S,8aR-octahydro-6,7-epoxy-1,4:5,8-dimethanonaphthalene **D276**
 hexachlorophane **H41**
 hexachlorophene **H41**
 hexachloroplatinic acid **C261**
 hexachloro-2-propanone **H32**
 1,1,1,3,3,3-hexachloro-2-propanone **H32**
 hexachloropropene **H42**
 1,1,2,3,3,3-hexachloro-1-propene **H42**
 hexachloropropylene **H42**
 4,5,6,7,8,8-hexachloro-3a,4,7,7a-tetrahydro-4,7-methanoisobenzofuran-1,3-dione **C123**
 (1,4,5,6,7,7-hexachloro-8,9,10-trinorborene-5-en-2,3-ylenebismethylene) sulfite **E19**
 hexacid C-7 **H22**
 hexaconazole **H43**
 1-hexadecanol **C102**
 hexadecene epoxide **E37**
N-hexadecyl-*N,N*-dimethylbenzenemethanaminium chloride **C103**
 hexadecylpyridinium chloride **C104**
 hexadecyltrimethylammonium bromide **C105**
 (*E,E*)-2,4-hexadienoic acid **S102**
 2,4-hexadienoic acid, potassium salt **P263**
 2,4-hexadienoic acid, sodium salt, *E,E*- **S91**
 hexadimethrine bromide **I56**
 hexadrin **E25**
 hexadrol **D62**
 hexaethyl tetraphosphate **H44**
 Hexaferb **F30**
 hexafluoroacetic anhydride **T291**
 hexafluoroacetone **H45**
 hexafluorodiethylnitrosamine **N145**
 hexafluoroethane **H46**
 hexafluoroisopropanol **H47**
 1,1,1,3,3,3-hexafluoro-2-propanol **H47**
 1,1,1,3,3,3-hexafluoro-2-propanone **H45**
 hexafluoropropene **H48**
 1,1,2,3,3,3-hexafluoropropene **H48**

hexafluoropropylene **H48**
 hexafluorosilicate(2-) **F73**
 hexafluorosilicate(2-) magnesium(1:1) **M4**
 hexafluosilic acid **F74**
 hexafor **H9**
 hexahydroaniline **C514**
 hexahydroazepine **H56**
 hexahydro-2*H*-azepine-2-one **C55**
N-[[[(hexahydro-1*H*-azepin-1-yl)amino]carbonyl]-4-methylbenzenesulfonamide **T170**
 1-(hexahydro-1*H*-azepin-1-yl)-3-(*p*-tolysulfonyl)urea **T170**
 hexahydrobenzene **C507**
 hexahydrocresol **M198**
 hexahydro-*p*-cresol **M201**
 hexahydro-1,4-diazine **P200**
 (E)-3,4,5,6,9,10-hexahydro-14,16-dihydroxy-3-methyl-1*H*-2-benzoxacyclotetradecin-1,7(8*H*)-dione **Z1**
 hexahydro-3*a*,7*a*-dimethyl-4,7-epoxyisobenzofuran-1,3-dione **C54**
 (2*α*,6*α*,11*R*^{*})-1,2,3,4,5,6-hexahydro-6,11-dimethyl-3-(3-methyl-2-butenyl)-2,6-methano-3-benzazocin-8-ol **P42**
 hexahydro-1,4-dinitroso-1*H*-1,4-diazepine **D494**
 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylcyclopenta[*g*]-2-benzopyran **G2**
 2,3,6*α*,8,9,9*α*-hexahydro-4-methoxycyclopenta[*c*]-furo[3',2':4,5]furo[2,3-*h*][1]benzopyran-1,11-dione **A54**
 3,4,7*α*,9,10,10*α*-hexahydro-5-methoxy-1*H*,12*H*-furo[3',2':4,5]furo[2,3-*h*]pyrano[3,4-*c*][1]benzopyran-1,12-dione **A56**
 hexahydromethylphenol **M198**
 hexahydro-1-methyl-4-phenyl-1*H*-azepine-4-carboxylic acid, ethyl ester **E73**
 hexahydro-*N*-nitrosopyridine **N172**
 (3*aS*-(3*a*-*α*-4-*β*,6*a*-*α*)-hexahydro-2-oxo-1*H*-thieno[3,4-*d*]imidazole-4-pentanoic acid **B112**
 hexahydrophenol **C508**
 hexahydrophthalic acid **H49**
cis-hexahydrophthalic anhydride **H50**
 hexahydropyrazine **P200**
 hexahydropyridine **P201**
 hexahydrothymol **M54**
 hexahydrotoluene **M197**
 (3*aS*-*cis*)-1,2,3,3*a*,8,8*a*-hexahydro-1,3*a*,8-trimethylpyrrolo-[2,3-*b*]indol-5-ol methylcarbamate (ester) **P178**
 hexahydro-1,3,5-trinitro-1,3,5-triazine **R2**
 hexahydro-1,3,5-tris(2-hydroxyethyl)-*s*-triazine **H51**
 (2*β*,3*β*,5*β*,22*R*)-2,3,14,20,22,25-hexahydroxycholest-7-en-6-one **E1**
 2,2,4,4,6,6-hexakis(1-aziridinyl)-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine **A229**
 hexakis(1-aziridinyl)phosphonitrile **A229**
 hexaldehyde **H59**
 hexalin **C508**
 hexametapol **H58**
 hexamethyldisilazane **H52**
 hexamethyldisiloxane **H53**
 hexamethylenamine **H57**
 hexamethylene **C507**
 1,1'-hexamethylenebis[5-(4-chlorophenyl)biguanide] **C130**
 hexamethylenediamine **H54**
 hexamethylene diisocyanate **H55**
 hexamethylene glycol diacrylate **H61**
 hexamethyleneimine **H56**
 hexamethylenetetramine **H57**
 hexamethylphosphoramidate **H58**
 hexamethylphosphoric triamide **H58**
 hexamethylsilazane **H52**
 hexamethylsilylamine **H52**
 hexamic acid **C495**
 hexamine **H57**
 hexanal **H59**
 5-hexanal, 2,6-epoxy **A36**
 hexanaphthylene **C511**
 hexanaphthene **C507**
 hexane **H60**
n-hexane **H60**
 1,6-hexanediamine **H54**
 hexane 1,6-diisocyanate **H55**
 hexanedinitrile **A49**
 hexanedioic acid **A48**
 hexanedioic acid, bis[2-(2-butoxyethoxy)ethyl] ester **D139**
 hexanedioic acid, bis(2-ethylhexyl) ester **D514**
 hexanedioic acid, bis(1-methylethyl) ester **D357**
 hexanedioic acid, bis(2-methylpropyl) ester **D351**
 hexanedioic acid, dibutyl ester **D140**
 hexanedioic acid, diethyl ester **D287**
 hexanedioic acid dinitrile **A49**
 hexanedioic acid, dioctyl ester **D513**
 1,6-hexanediol diacrylate **H61**
 2,5-hexanedione **H62**
 1,2,3,4,5,6-hexanehexol **M28**
 1-hexanethiol **H63**
 Hexaniat **I38**
 2,4,6,2',4',6'-hexanitrodiphenylamine **D550**
 Hexanium **E16**
 hexanoic acid **H64**
 1-hexanol **H65**
 2-hexanol **H66**
 hexan-2-one **H67**
 2-hexanone **H67**
 3-hexanone **H68**
 hexapropyl-distannoxane **T344**
 hexasodium hexametaphosphate **S69**
 Hexason **P118**
 hexazane **P201**
 hexazinone **H69**
 1-hexene **H70**
 1-hexene epoxide **E38**
 1,2-hexene oxide **E38**
 1-hexene oxide **E38**
 1-hexen-3-ol **H71**
 2-hexenol **H72**
cis-3-hexenol **H74**
 (E)-2-hexen-1-ol **H72**

(E)-3-hexen-1-ol **H73**
trans-2-hexenol **H72**
trans-3-hexenol **H73**
 (Z)-3-hexen-1-ol **H74**
 δ - $\Delta\alpha,\beta$ -hexenolactone **P12**
 2-hexen-5,1-olide **P12**
 hexeral(barbiturate) **H76**
 hexetidine **H75**
 Hexevax **C84**
 Hexilur **L34**
 hexobarbital **H76**
 hexobarbitone **H76**
 Hexocil **H75**
 hexogen **R2**
n-hexoic acid **H64**
 hexone **M241**
 hexophene **H41**
 hexyl **D550**
sec-hexyl acetate **H77**
 hexyl acrylate **H78**
n-hexyl alcohol **H65**
 hexylbenzene **P107**
 hexylene **H70**
 hexylene glycol **M275**
 hexyl mercaptan **H63**
 hexyl methyl ketone **O16**
 hexyl 2-propenoate **H78**
 hexylthiocarbam **C498**
 hexyltrichlorosilane **H79**
 hexythiazox **H80**
 HFIP **H47**
 HHDN **A65**
 Hi-Cane **C479**
 Hidkitex DF **S50**
 Hi-Dry **T64**
 hi-flash naphtha **N5**
 Hildan **E20**
 Hildan **E19**
 Hiltaklor **B196**
 Hiltonil Fast Blue B Base **D95**
 Hiltonil Fast Scarlet 2G Base **D180**
 Hinorabacide **E2**
 Hinosan **E2**
 hippuric acid **H81**
 hiptagenic acid **N140**
 Hispacet Fast Yellow G **C410**
 Histadyl **M117**
 Histidyl **M118**
 Hitox **T165**
 Hi-A-vita **R7**
 HMDA **H54**
 HMDI **M211**
 HMDI **H55**
 HMDS **H52**
 HMPA **H58**
 HMT **H57**
 HN1 **H82**
 HNE **H114**
 HN₂ oxide mustard **M39**
 HNU **H111**
 Hoe 2960 **T205**
 Hoegrass **D259**
 Hoelon **D259**
 HOK 7501 **M33**
 holmium **H83**
 Hombitan **T165**
 homidium bromide **E65**
 homopiperidine **H56**
 homosterone **T38**
 Hordaflex **C132**
 Hormex **I34**
 Hormodiu **I34**
 Hostafume **P305**
 Hostaquick **H29**
 Hostathion **T205**
 HS **H89**
 HTG 10 **C319**
 HTH **C34**
 Huile H50 **T139**
 Hustisol **G47**
 Hyamine 1622 **B51**
 hybar X **U8**
 hycanthon **H84**
 hycanthone **H84**
 hycar **P222**
 Hycortol **H95**
 Hydan **D205**
 Hydantoin **P142**
 hydantoin, 1,3-dichloro-5,5-dimethyl- **D205**
 hydracrylic acid, β -lactone **P308**
 hydralazine chloride **H85**
 hydralazine hydrochloride **H85**
 hydramethylnon **H86**
 hydrargyrum **M64**
 hydrated lime **C33**
 hydrated potassium sodium calcium magnesium
 aluminium silicate **E45**
 hydrazidodicarbonthioamide **D573**
 hydrazine **H87**
 hydrazine-*N,N'*-bisthiocarbonamide **D573**
 hydrazinecarbohydrazonothioic acid **T124**
 hydrazinecarbothiamide **T144**
 hydrazinecarbothioamide 2,2'-methylenebis- **M215**
 hydrazinecarboxamide monohydrochloride **S22**
 1,2-hydrazinedicarbthioamide **D573**
 hydrazine hydrate **H88**
 hydrazine hydrogen sulfate **H89**
 hydrazine monosulfate **H89**
 hydrazine sulfate **H89**
 hydrazinium sulfate **H89**
 2-hydrazino-4-(4-aminophenyl)thiazole **H90**
 2-hydrazino-4-(*p*-aminophenyl)thiazole **H90**
 hydrazinobenzene **P108**
 hydrazinoethanol **H91**

2-hydrazinoethanol **H91**
 2-hydrazinoethyl alcohol **H91**
o-hydrazinonitrobenzene **N135**
p-hydrazinonitrobenzene **N136**
 2-hydrazino-4-(5-nitro-2-furanyl)thiazole **H92**
 2-hydrazino-4-(5-nitro-2-furyl)thiazole **H92**
 2-hydrazino-4-(*p*-nitrophenyl)thiazole **H93**
 1-hydrazino-2-phenylethane hydrogen sulfate **P64**
 1-hydrazinophthalazine hydrochloride **H85**
 hydrazobenzene **D546**
 hydrazoic acid **H97**
 hydrazomethane **D421**
 hydrazonium sulfate **H89**
 hydrindene **I17**
 hydrindonaphthene **I17**
 1-hydrindone **I20**
 α -hydrindone **I20**
 β -hydrindone **I21**
 hydriodic acid **H102**
 hydriodic ether **I49**
 hydroazoethen **D306**
 hydrobromic acid **H98**
 hydrobromic ether **B175**
 hydrocarbon wax **P7**
 hydrocarbon waxes, chlorinated **C132**
 Hydrocerol A **C352**
 hydrochloric acid **H99**
 hydrochloric ether **C196**
 hydrochlorothiazide **H94**
 hydrochlorous acid, sodium salt, pentahydrate **S75**
 hydrocinnamaldehyde, *p*-*tert*-butyl- α -methyl- **L44**
 hydrocortisone **H95**
 Hydrocortone **H95**
 hydrocyanic acid **H100**
 hydrocyanic acid, potassium salt **P245**
 hydrocyanic ether **P312**
 Hydrodiuril **H94**
 hydrofluoboric acid **F46**
 hydrofluoric acid gas **H101**
 hydrogen **H96**
 hydrogen arsenide **A246**
 hydrogen azide **H97**
 hydrogen bromide **H98**
 hydrogen carboxylic acid **F104**
 hydrogen chloride **H99**
 hydrogen cyanamide **C479**
 hydrogen cyanide **H100**
 hydrogen dioxide **H103**
 hydrogen fluoride **H101**
 hydrogen hexachloroplatinate(IV) **C261**
 hydrogen hexafluorosilicate **F74**
 hydrogen iodide **H102**
 hydrogen nitrate **N68**
 hydrogen peroxide **H103**
 hydrogen phosphide **P155**
 hydrogen potassium fluoride **P252**
 hydrogen selenide **H104**
 hydrogen sodium sulfide **S72**
 hydrogen sodium sulfite **S48**
 hydrogen sulfide **H105**
 hydrogen tetrafluoroborate **F46**
 Hydrogloss **K2**
 α -hydro- ω -hydroxypoly(oxy-1,2-ethanediyl) **P225**
 Hydrol SW **O20**
 8-hydromirex **P169**
 hydronitric acid **H97**
 Hydronol **I137**
 hydroprene **H106**
 2-hydroproperoxy-2-methylpropane **B261**
O-hydroquinine dimethyl ether **V18**
 hydroquinone **H107**
m-hydroquinone **R5**
o-hydroquinone **C95**
 hydroquinone, *tert*-butyl **B262**
 hydroquinone methyl ether **M144**
 Hydro-Saluric **H94**
 Hydrosekt **B223**
 hydrosilicofluoric acid **F74**
 hydrosulfuric acid **H105**
 hydrotalcite **H108**
 Hydrothol **E23**
 Hydroton **C318**
 Hydrovit A **V40**
 2-(*N*-hydroxyacetamido)fluorene **H109**
 4-hydroxyacetanilide **P6**
 hydroxyacetoneitrile **G37**
N-hydroxy-2-acetylaminofluorene **H109**
N-hydroxy-*N*-acetyl-2-aminofluorene **H109**
 4-hydroxyafatoxin B₁ **A57**
 hydroxyamine **H112**
 α -hydroxy- β -aminopropylbenzene hydrochloride **N203**
 17 β -hydroxyandrost-4-en-3-one **T38**
 17 β -hydroxy- Δ^4 -androst-3-one **T38**
 2-hydroxyaniline **A142**
 3-hydroxyaniline **A143**
p-hydroxyaniline **A144**
 4-hydroxy-*m*-anisaldehyde **V17**
 4-hydroxyazobenzene **C425**
 2-hydroxybenzaldehyde **S4**
o-hydroxybenzaldehyde **S4**
 2-hydroxybenzamide **S5**
 hydroxybenzene **P80**
 (\pm)- α -hydroxybenzeneacetic acid **M20**
 α -hydroxybenzeneacetic acid, 3,3,5-trimethylcyclohexyl ester **C496**
p-hydroxybenzenesulfonic acid, zinc salt **Z13**
 2-hydroxybenzoic acid **S6**
o-hydroxybenzoic acid **S6**
p-hydroxybenzoic acid, ethyl ester **E158**
 2-hydroxybenzoic acid, mercury complex **M84**
 4-hydroxybenzoic acid, methyl ester **M272**
 2-hydroxybenzoic acid, phenyl ester **P132**
 4-hydroxybenzoic acid, propyl ester **P336**
 hydroxybenzopyridine **H119**

α -hydroxybenzyl phenyl ketone **B64**
 3-hydroxybiphenyl **P126**
p-hydroxybiphenyl **P127**
endo-2-hydroxybornane **B143**
 hydroxybrasilin **H14**
 hydroxybrazilin **H14**
 3-hydroxybutanal **A63**
 1-hydroxybutane **B212**
 2-hydroxybutane **B213**
 hydroxybutanedioic acid **M15**
 4-hydroxy-1-butanefulfonic acid **B210**
 3-hydroxybutanoic acid β -lactone **B287**
 1-hydroxy-2-butene **C470**
 3-hydroxy-1-butene **B220**
 2-hydroxy-3-butoxypropane **B231**
 1-hydroxy-4-*tert*-butylbenzene **B276**
 3-hydroxybutyraldehyde **A63**
 β -hydroxybutyraldehyde **A63**
 3-hydroxybutyric acid lactone **B287**
 β -hydroxybutyric acid lactone **B287**
 γ -hydroxybutyrolactone **B288**
 hydroxy-*o*-carboxyphenylfluorone, sodium salt **C399**
 2-hydroxychlorobenzene **C239**
 3-hydroxychlorobenzene **C240**
 4-hydroxychlorobenzene **C241**
 3-hydroxy-3-(4-chloro-3-sulfonylphenyl)phthalimidine **C318**
 3 α -hydroxycholanolic acid **L56**
 3-hydroxy-cholan-24-oic acid, (3 α ,5 β)- **L56**
 3 α -hydroxy-5 β -cholan-24-oic acid **L56**
o-hydroxycinnamic acid lactone **C447**
 17-hydroxycorticosterone **H95**
 4-hydroxycrotonic acid γ -lactone **F124**
 γ -hydroxycrotonic acid lactone **F124**
 α -hydroxycumene **P131**
 hydroxycyclopentane **C524**
 14-hydroxydaunomycin **D596**
 14-hydroxydaunomycin hydrochloride **D597**
 hydroxydecane **D42**
 1-hydroxy-2,4-diaminobenzene **D81**
 4-hydroxy-3,5-diiodobenzonitrile **I59**
o-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-L-tyrosine **T156**
 hydroxydimethylarsine oxide **C1**
 1-hydroxy-2,4-dimethylbenzene **X10**
 1-hydroxy-2,4-dinitrobenzene **D486**
 1-hydroxy-2,5-dinitrobenzene **D487**
 1-hydroxy-2,6-dinitrobenzene **D488**
 2-hydroxydiphenol **P125**
 4-hydroxydiphenyl ether **P87**
p-hydroxydiphenyl ether **P87**
 20-hydroxyecdysone **E1**
 9-hydroxyellipticine **H110**
 3-hydroxyestra-1,3,5(10),7-tetraen-17-one **E41**
 3-hydroxyestra-1,3,5(10)-trien-17-one **E53**
 hydroxyethanediphosphonic acid **E183**
 2-hydroxyethanol **E116**
 hydroxyethene **V27**
 2-hydroxyethyl acetate **E117**
 2-hydroxyethylamine **E62**
 2,2'-[[4-[(2-hydroxyethyl)amino]-3-nitrophenyl]imino]diethanol **H8**
 α -hydroxyethylbenzene **P68**
 β -hydroxyethylbenzene **P67**
 (2-hydroxyethyl)dimethylamine **D388**
 hydroxyethylene **V27**
 1-hydroxyethyl-2-heptadecylglyoxalidine **H17**
 (2-hydroxyethyl)hydrazine **H91**
 (β -hydroxyethyl)hydrazine **H91**
 2-hydroxyethyl 2-hydroxybenzoate **G38**
 (1-hydroxyethylidene)bis-[phosphonic acid] **E183**
 (hydroxyethylidene)diphosphonic acid **E183**
 (1-hydroxyethylidene)-1,1-diphosphonic acid **E183**
 3- β -hydroxyethylindole **T370**
 2-hydroxyethyl mercaptan **M62**
 (2-hydroxyethyl)methylamine **M155**
 1-(2-hydroxyethyl)-2-methyl-5-nitroimidazole **M327**
 1-(2-hydroxyethyl)-1-nitrosourea **H111**
 β -hydroxyethyl phenyl ether **P86**
 2-hydroxyethyl salicylate **G38**
 2-hydroxyethyl sulfide **T129**
 β -hydroxyethyl sulfide **T129**
 4-(α -hydroxyethyl)toluene **D402**
 (2-hydroxyethyl)trimethylammonium **C326**
 (2-hydroxyethyl)trimethylammonium salicylate **C327**
 9-hydroxyfluorene-9-carboxylic acid, butyl ester **F85**
 9-hydroxy-9*H*-fluorene-9-carboxylic acid, butyl ester **F85**
 4-hydroxy-4*H*-furo[3,2-*c*]pyran-2(6*H*)-one **P16**
 1-hydroxyhexane **H65**
 5-hydroxy-2-hexenoic acid lactone **P12**
 5-hydroxyhydrindene **I19**
 1-hydroxy-1'-hydroperoxydicyclohexyl peroxide **C510**
 17-hydroxy-2-(hydroxymethylene)-17- β -methyl-5 α -androstane-3-one **O62**
 5-hydroxyindan **I19**
 2-hydroxyisobutyronitrile **A18**
 α -hydroxyisobutyronitrile **A18**
 4-hydroxy-2-keto-4-methylpentane **D65**
 hydroxylamine **H112**
 2-hydroxymesitylene **T322**
 4-hydroxy-3-methoxybenzaldehyde **V17**
 6-hydroxy-7-methoxy-5-benzofuranacrylic acid δ -lactone **M129**
 3-hydroxy-4-[(2-methoxy-5-nitrophenyl)azo]-*N*-(3-nitrophenyl)-2-naphthalenecarboxamide **C417**
 2-hydroxy-3-(*o*-methoxyphenoxy)propyl 1-carbamate **M125**
 4-hydroxy-3-methoxy-1-propenylbenzene **I102**
N-(hydroxymethyl)acrylamide **H113**
 (*R*)-3-hydroxy- α -[(methylamino)methyl]benzenemethanol **P106**
 1-hydroxy-2-methylbenzene **C458**
 α -(hydroxymethyl)benzeneacetic acid, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester **H124**
N-(hydroxymethyl)-2-chloracetamide **C204**

3-hydroxymethylchrysazin **A95**
 7-hydroxy-4-methylcoumarin, *O*-ester with *O,O*-diethyl phosphorothioate **D309**
 2-hydroxy-3-methyl-2-cyclopenten-1-one **M31**
 5-[1-hydroxy-2-[(1-methylethyl)amino]ethyl]-1,3-benzenediol **O33**
 2-hydroxymethylfuran **F127**
 3-(hydroxymethyl)-*n*-heptan-4-ol **E126**
 3-hydroxy-5-methylisoxazole **H121**
 3-hydroxy-*N*-methylmorphinan (+)-form, methyl ether **D63**
 5-hydroxy-2-methyl-1,4-naphthalenedione **P216**
 5-hydroxy-2-methyl-1,4-naphthoquinone **P216**
 hydroxymethylnitrile **G37**
 2-hydroxy-3-methylnitrobenzene **N108**
p-(hydroxymethyl)nitrobenzene **N96**
 2-(hydroxymethyl)-2-nitro-1,3-propanediol **T357**
 2-(hydroxymethyl)oxirane **G28**
 3-hydroxy-3-methylpentane **M279**
 4-hydroxy-4-methyl-2-pentanone **D65**
 4-hydroxy-4-methylpentan-2-one **D65**
 4-hydroxy-4-methyl-2-pentenoic acid γ -lactone **D417**
 12'-hydroxy-2'-methyl-5' α -(phenylmethyl)ergotamane-3',6',18-trione tartrate **E44**
 4-[(hydroxymethyl)phosphinoyl]-DL-homoalanine **G18**
 4-[hydroxy(methyl)phosphinoyl]-L-homoalanyl-L-alanyl-L-alanine **B110**
 4-(hydroxymethylphosphinyl)-L-2-aminobutanoyl-L-alanyl-L-alanine **B110**
 17-hydroxy-6-methylpregna-4,6-diene-3,20-dione acetate **M44**
N-(hydroxymethyl)-2-propenamide **H113**
 3-hydroxy-2-methylpropene **M289**
 5-hydroxy-6-methyl-3,4-pyridinedimethanol **P358**
 5-hydroxy-6-methyl-3,4-pyridinedimethanol hydrochloride **P359**
 12-hydroxy-4-methyl-4,8-secosenecionan-8,11,16-trione **S23**
 3-hydroxy- α -methyl-L-tyrosine, **M208**
 hydroxymycin **N38**
 1-hydroxynaphthalene **N17**
 2-hydroxynaphthalene **N18**
 α -hydroxynaphthalene **N17**
 4-[(2-hydroxy-1-naphthalenyl)azo]-1-naphthalenesulfonic acid, monosodium salt **C397**
 2-hydroxy-3-naphthoanilide **N19**
p-[(2-hydroxy-1-naphthyl)azo]benzenesulfonic acid, sodium salt **C391**
 2-hydroxy-4-nitroaniline **A139**
 2-hydroxy-5-nitroaniline **A138**
 4-hydroxy-3-nitroaniline **A140**
 2-hydroxynitrobenzene **N130**
 3-hydroxynitrobenzene **N131**
 4-hydroxynitrobenzene **N132**
N-hydroxy-*N*-nitrosobenzenamine, ammonium salt **C476**
 2-hydroxy-4-nitrotoluene **N106**
 3-hydroxy-2-nitrotoluene **N103**
 4-hydroxy-3-nitrotoluene **N104**
 5-hydroxy-2-nitrotoluene **N105**
 2-hydroxy-3-nitrotoluol **N108**
 4-hydroxy-2-nonenal **H114**
 17-hydroxy-19-nor-17 α -pregn-5(10)-en-20-yn-3-one **N205**
 (17 α)-17-hydroxy-19-norpregn-4-en-20-yn-3-one **N204**
 (17 α)-17-hydroxy-19-norpregn-5(10)-en-20-yn-3-one **N205**
 1-hydroxyoctane **O13**
 2-hydroxy-*n*-octane **O14**
 4-hydroxy-3-[3-oxo-1-(4-chlorophenyl)-butyl]coumarin **C445**
 4-hydroxy-3-(3-oxo-1-phenylbutyl)-2*H*-1-benzopyran-2-one **W1**
 (*R*)-4-hydroxy-3-(3-oxo-1-phenylbutyl)-2*H*-1-benzopyran-2-one **W2**
 4-hydroxy-3-(3-oxo-1-phenylbutyl)coumarin **W1**
 6-(10-hydroxy-6-oxo-*trans*-1-undecenyl)- β -resorcylic acid-*n*-lactone **Z1**
 4-hydroxypentanoic acid lactone **V3**
 4-hydroxyphenethylamine **T375**
 2-hydroxyphenol **C95**
 3-hydroxyphenol **R5**
m-hydroxyphenol **R5**
o-hydroxyphenol **C95**
p-hydroxyphenol **H107**
 α -(4-hydroxyphenol)- β -aminoethane **T375**
 7-hydroxy-3*H*-phenoxazin-3-one, ethyl ether **E86**
 1-hydroxy-2-phenoxyethane **P86**
N-(4-hydroxyphenyl)acetamide **P6**
 2-hydroxy-2-phenylacetophenone **B64**
 α -hydroxy- α -phenylacetophenone **B64**
p-hydroxyphenylbutazone **O63**
N'-(*m*-hydroxyphenyl)-*N,N*-dimethylformamidin-methylcarbamate ester **F102**
 (4-hydroxyphenyl)ethane **E162**
 (*p*-hydroxyphenyl)ethane **E162**
 (6*R*)-6-[α -D-(14-hydroxyphenyl)glycylamino]penicillanic acid **A192**
 hydroxyphenylmercury **P119**
 hydroxyphenylmercury mixture with (*nitrate*-*O*)phenylmercury **P120**
 3-hydroxy-*N*-phenyl-2-naphthalenecarboxamide **N19**
 hydroxypiracyl alcohol **N40**
 17-hydroxypregn-4-ene-3,20-dione **H115**
 3-hydroxypregn-5-en-20-one **P270**
 hydroxyprogesterone **H115**
 17 α -hydroxyprogesterone **H115**
 1-hydroxypropane **P296**
 5,5'-[(2-hydroxy-1,3-propanediyl)bis(oxy)]bis[4-oxo-4*H*-1-benzopyran-2-carboxylic acid] **S57**
 3-hydroxy-1-propanesulfonic acid sultone **P293**
 2-hydroxypropanoic acid, butyl ester **B266**
 2-hydroxypropanol **P327**
 3-hydroxypropene **A73**
 2-hydroxypropionic acid **L1**
 3-hydroxypropionic acid lactone **P308**
 2-hydroxypropionitrile **L2**

2-hydroxypropyl acrylate **H116**
 2-hydroxypropylamine **A148**
 3-hydroxypropylene oxide **G28**
 2-hydroxypropyl methacrylate **H117**
 β -hydroxypropyl methacrylate **H117**
 3-hydroxy-1-propyne **P301**
 3-hydroxypseudocumene **T321**
 6-hydroxypseudocumene **T320**
 4-hydroxypyrazolo[3,4-d]pyrimidine **A70**
 6-hydroxy-2*H*-pyridazin-3-one **M14**
 6-hydroxy-3(2*H*)-pyridazinone **M14**
 2-hydroxy-5-[[4-[(2-pyridinylamino)sulfonyl]phenyl]azo]benzoic acid **S140**
 5-(α -hydroxy- α -2-pyridylbenzyl)-7-(α -2-pyridylbenzylidene)-5-norbornene-2,3-dicarboximide **N201**
 2-hydroxyquinoline **H118**
 8-hydroxyquinoline **H119**
 hydroxyquinoline sulfate **H120**
 8-hydroxyquinoline sulfate **H120**
 hydroxysuccinic acid **M15**
 3-hydroxy-4-[(4-sulfo-1-naphthalenyl)azo]-2,7-naphthalenedisulfonic acid trisodium salt **A108**
 7-hydroxy-8-[(4-sulfo-1-naphthyl)azo]-1,3-naphthalenedisulfonic acid, trisodium salt **C394**
 6-hydroxy-5-[(4-sulfo-1-naphthyl)azo]-2-naphthalenesulfonic acid, disodium salt **C415**
 5-hydroxytetracycline **O64**
 4-hydroxy-3-(1,2,3,4-tetrahydro-1-naphthalenyl)-2*H*-1-benzopyran-2-one **C448**
 4-hydroxy-3-(1,2,3,4-tetrahydro-1-naphthyl)coumarin **C448**
 4-hydroxy-3-[1,2,3,4-tetrahydro-3-[4-(4-trifluoromethylbenzyloxy)phenyl]-1-naphthyl]coumarin **F37**
 4-hydroxy-3-[1,2,3,4-tetrahydro-3-[4-[[4-(trifluoromethyl)phenyl]methoxy]phenyl]-1-naphthalenyl]-2*H*-1-benzopyran-2-one **F37**
 4-hydroxy-3-(α -tetralyl)coumarin **C448**
 7-hydroxy-3,4-tetramethylenecoumarin *O,O*-diethyl thiophosphate **C450**
 hydroxytoluene **C456**
 2-hydroxytoluene **B89**
 3-hydroxytoluene **C457**
 α -hydroxytoluene **B89**
o-hydroxytoluene **C458**
p-hydroxytoluene **C459**
 4'-((6-hydroxy-*m*-tolyl)azo)acetanilide **C410**
 2-hydroxytriethylamine **D289**
 4-hydroxy- $\alpha,\alpha,4$ -trimethylcyclohexanemethanol **T32**
 2-hydroxy-*N,N,N*-trimethylethanaminium salt with 2-hydroxybenzoic acid (1:1) **C327**
 3-hydroxy-4-[(2,4,5-trimethylphenyl)azo]-2,7-naphthalenedisulfonic acid, disodium salt **C414**
 2-hydroxy-1,3,5-trinitrobenzene **P187**
 hydroxytriphenylstannane **F26**
 3-hydroxytyramine **D595**
 3-hydroxy-L-tyrosine **L37**
 4-hydroxyvaleric acid lactone **V3**

3-hydroxy-4(2,4-xylylazo)-3,7-naphthalenedisulfonic acid, disodium salt **C395**
 hydrozoethane **D306**
 Hyfatol 16-98 **C102**
 Hyfatol 18-95 **S113**
 Hylemox **E68**
 Hymecromone *O,O*-diethyl phosphorothioate **D309**
 hymexazol **H121**
 Hyminal **M119**
 hyoscine **H122**
 hyoscine bromide **H123**
 hyoscine hydrobromide **H123**
 hyoscyamine **H124**
 hyosol **H122**
 DL-hyoxyomene **A253**
 Hypatrol **Q3**
 Hyperazin **H85**
 Hyperkil **E42**
 hypochlorous acid, calcium salt **C34**
 hypochlorous acid, lithium salt **L55**
 Hypodermacid **T225**
 hyponitrous acid anhydride **N183**
 Hypothiazide **H94**
 hypoxanthine nucleoside **I36**
 hypoxanthine riboside **I36**
 hypoxanthosine **I36**
 HyPure L **L55**
 Hystore **T14**
 Hytox **I116**
 Hyvar X **B151**
 IAA **I32**
 IAN **I33**
 IBZ **I1**
 IBA **I34**
 ibenzmethylin hydrochloride **I1**
 Ibifur **F122**
 Ibis **E63**
 IBP **I61**
 Ibufen **I2**
 ibuprofen **I2**
 ice spar **C472**
 ice stone **C472**
 ICI 35868 **P314**
 ICI-PP 333 **P1**
 Iconol NP 100 **N196**
 IDA **I11**
 IDPN **I13**
 Idrorame **B142**
 Iduridin **I48**
 IFN- α **I39**
 ifosfamide **I3**
 Ignite **G18**
 Igram **T25**
 Ikkokuso **C106**
 IL6001 **T328**
 Ilexan E **E116**
 Illoxan **D259**

imazalil **I4**
 Imazamethabenz **I5**
 imazamethabenz-methyl **I5**
 imazapyr **I6**
 imazethapyr **I7**
 Imferon **I70**
 IMI 115 **T164**
 imidacloprid **I8**
 Imidan **P153**
 Imidathion **P153**
 imidazole **I9**
 1*H*-imidazole **I9**
 imidazole, 1-butyl **B263**
 1*H*-imidazole, 1-butyl **B263**
 2-imidazolidinethione **E122**
 2,4-imidazolinedione, 1,3-dichloro-5,5-dimethyl- **D205**
 7*H*-imidazo[4,5-*d*]pyrimidine **P346**
 imidocarbonic acid, phosphonodithio-, cyclic ethylene *P,P*-diethyl ester **P151**
 imidocarbonic acid, phosphonodithio-, cyclic propylene **M56**
 4,4'-(imidocarbonyl)bis(*N,N*-dimethylaniline) **A254**
 imidole **P366**
 Imifen **I5**
 iminobis(acetic acid) **I11**
 2,2'-iminobis(ethanol) **D281**
 iminobis-3-isopropylamine **N208**
 3,3'-iminobis(propanenitrile) **I13**
 1,1'-iminobis-2-propanol **D356**
 3,3'-iminobis(1-propanol) dimethanesulfonate hydrochloride **I16**
 iminobispropylamine **N208**
 3,3'-iminobis(propylamine), *N*-(3-aminopropyl)-1,3-propanediamine **N208**
 iminoctadine **I10**
 iminodiacetic acid **I11**
 iminodibenzyl **I12**
 2,2'-iminodiethanol **D281**
 2,2'-iminodiethylamine **D303**
 1,1'-iminodi(octamethylene)diguanidinium triacetate **I10**
 1,1'-iminodi-2-propanol **D356**
 1,1'-iminodipropan-2-ol **D356**
 3,3'-iminodipropionitrile **I13**
 β,β' -iminodipropionitrile **I13**
 (1-iminoethyl)-phosphoramidothioic acid, *O,O*-bis(4-chlorophenyl)ester **P148**
 imipramine **I14**
 imipramine hydrochloride **I15**
 Impact **F93**
 Imperial Green **P15**
 Imposil **I70**
 improsulfan hydrochloride **I16**
 Improval **B245**
 Imutex **I9**
 IN 511 **P140**
 Inacid **I35**
 Incidal **M36**
 Inco **C376**
 incorporation factor **G25**
 Incromide CA **C381**
 Indalca A G **G51**
 Indalca PR90 **L57**
 indan **I17**
 1,3-indandione **I18**
 5-indanol **I19**
 indanone **I20**
 1-indanone **I20**
 2-indanone **I21**
 α -indanone **I20**
 indazole **I22**
 1*H*-indazole **I22**
 inden **I23**
 indene **I23**
 1*H*-indene **I23**
 1*H*-indene, 2,3-dihydro-5-methyl **M237**
 Indene, 2,3-dimethyl- **D425**
 1*H*-indene-1,3(2*H*)-dione **I18**
 indeno[1,2,3-*cd*]pyrene **I24**
 Indian gum **G53**
 Indian saffron **C478**
 Indian tragacanth gum **K3**
 Indigo **I25**
 Indigo Blue **I25**
 Indigo Blue 2B **C404**
 Indigo Carmine **I26**
 indium **I27**
 Indium chloride (InCl₃) **I29**
 indium phosphide **I28**
 indium trichloride **I29**
 Indocin **I35**
 Indocyanine Green **I30**
 indole **I31**
 1*H*-indole **I31**
 indoleacetic acid **I32**
 indole-3-acetic acid **I32**
 1*H*-indole-3-acetic acid **I32**
 indoleacetoneitrile **I33**
 indole-3-acetonitrile **I33**
 1*H*-indole-3-acetonitrile **I33**
 3-indoleacetoneitrile **I33**
 1*H*-indole-3-butyric acid **I34**
 indole-3-butyric acid **I34**
 3-indolebutyric acid **I34**
 1*H*-indole, 7-chloro- **C205**
 1*H*-indole-2,3-dione **I78**
 1*H*-indole-3-ethanamine **T367**
 indole ethanol **T370**
 1*H*-indole-3-ethanol **T370**
 indol-3-ylacetic acid **I32**
 3-indolylacetoneitrile **I33**
 1- β -3-indolylalanine **T369**
 4-(indol-3-yl)butyric acid **I34**
 β -indolylbutyric acid **I34**
 3-indolylethanol **T370**

2-(3-indolyl)ethyl alcohol **T370**
 2-(3-indolyl)ethylamine **T367**
 Indomed **I35**
 Indomee **I35**
 indomethacin **I35**
 indonaphthene **I23**
 indone **I20**
 1-indone **I20**
 Indoptol **I35**
 Induclor **C34**
 Indulin A **L42**
 Infecundin **E28**
 Ingalite Fast Brilliant Blue-BL **P176**
 INH **I109**
 innesonal **Q3**
 Ino **I36**
 Inosie **I36**
 inosine **I36**
 inosital **I37**
 inositol **I37**
myo-inositol **I37**
D-chiro-inositol, 3-O-[2-amino-4-[(carboxyiminomethyl)-amino]-2,3,4,6-tetradeoxy- α -D-arabino-hexopyranosyl]-**K5**
myo-inositol hexakis(dihydrogen phosphate) **P180**
myo-inositol hexaphosphate **P180**
 inositolhexaphosphoric acid **P180**
myo-inositol hexa-3-pyridinecarboxylate **I38**
 inositol niacinate **I38**
 inositol nicotinate **I38**
 Insegar **F17**
 instrex **P231**
 Insulamina **L37**
 Intal **S57**
 Integral Rat **C448**
 Intense Blue **I26**
 interferon- α **I39**
 interferon A **I39**
 interferon alfa **I39**
 Interselect **H103**
 Intox **C118**
 Intrazol **C68**
 Intration **T134**
 iodic acid (HIO₃), potassium salt **P255**
 iodine **I40**
 iodine chloride **I41**
 iodine cyanide **C485**
 iodine monochloride **I41**
 iodoacetic acid **I42**
p-iodoaminobenzene **I44**
 3-iodoaniline **I43**
 4-iodoaniline **I44**
m-iodoaniline **I43**
p-iodoaniline **I44**
 3-iodobenzamine **I43**
 4-iodobenzamine **I44**
 2-iodobenzanilide **B31**
 iodobenzene **I45**
 1-iodobutane **I46**
 2-iodobutane **I47**
sec-iodobutane **I47**
 iodochlorine **I41**
 5-iodo-2'-deoxyuridine **I48**
 iododichloromethane **D220**
 iodoethane **I49**
 iodofenphos **I50**
 iodoform **I51**
 iodomethane **I52**
 1-iodo-2-methylpropane **I53**
 2-iodo-2-methylpropane **I54**
 4-iodophenol **I55**
p-iodophenol **I55**
 2-iodo-*N*-phenylbenzamide **B31**
 iodophos **I50**
 3-iodo-1-propene **A85**
 3-iodopropylene **A85**
 Ionamin **P88**
 6,3-ionene **I56**
 Ionol **B245**
 α -ionone **I57**
 β -ionone **I58**
 (*E*)- α -ionone **I57**
trans- α -ionone **I57**
 iopezite **P246**
 Iota **F92**
 ioxynil **I59**
 IPA **P297**
 ipecac, *C. ipecacuanha* **I60**
 ipecac syrup **I60**
 ipecacuanha **I60**
 Ipegol Co-630 **N196**
 IPO 10 **D460**
 Ipon **I133**
 IPP **D360**
 iprobenfos **I61**
 Iprodial **I62**
 iprodione **I62**
 iproniazid dihydrogen phosphate **I63**
 iproniazid phosphate **I63**
 Ircon **I72**
 Irenat **S83**
 iridium **I64**
 Iridium Black **I64**
 iridium chloride **I65**
 iridium tetrachloride **I65**
 Iridocin **E69**
 iron **I66**
 iron(II) ammonium sulfate **I67**
 iron carbonyl (Fe(CO)₅) **I75**
 (TB-5-11)-iron carbonyl (Fe(CO)₅) **I75**
 iron chloride **I69**
 iron(II) chloride **I68**
 iron(III) chloride **I69**
 iron(III) dextran **I70**

iron dichloride **I68**
 iron dimethyldithiocarbamate **F30**
 iron(III) fluoride **I71**
 iron(II) fumarate **I72**
 iron monosulfate **I76**
 iron(III) nitrate **I73**
 α -iron oxide **I74**
 γ -iron oxide **I74**
 iron(III) oxide **I74**
 iron pentacarbonyl **I75**
 iron perchloride **I69**
 iron persulfate **I77**
 iron protochloride **I68**
 iron sulfate (2:3) **I77**
 iron(II) sulfate **I76**
 iron(III) sulfate **I77**
 iron tersulfate **I77**
 iron trichloride **I69**
 iron trifluoride **I71**
 iron trinitrate **I73**
 Irtiran 3 **F80**
 Isarol **S139**
 isatic acid lactam **I78**
 isatin **I78**
 isatinic acid anhydride **I78**
 isazofos **I79**
 Isazophos **I79**
 Ismipur **M63**
 Ismotic **I137**
 isoacetophorone **I110**
 isoamyl acetate **I80**
 isoamyl alcohol **M174**
 isoamyl aldehyde **I140**
 isoamyl bromide **B179**
 isoamyl cyanide **I142**
 α -isoamylene **M175**
 β -isoamylene **A200**
 4-(β -isoamylene)-1,2-diphenyl-3,5-pyrazolidenedione
F29
 isoamyl ethanoate **I80**
 isoamyl hydride **M172**
 isoamyl methyl ketone **M233**
 isoamyl nitrite **I81**
 isoamylol **M174**
 isobenzan **I82**
 1,3-isobenzofurandione **P173**
cis-1,3-isobenzofurandione, hydro- **H50**
 1,3-isobenzofurandione, 3,4,7,7-tetrahydro- **T76**
 Isobide, 1,4:3,6-dianhydrosorbitol **I137**
 isoborneol acetate **I83**
 isobornyl acetate **I83**
 isobutanal **I97**
 isobutane **I84**
 isobutanoic acid **I98**
 isobutanol **I85**
 isobutenal **M103**
 isobutene **I86**
 isobutenylcarbinol **M177**
 isobutenyl chloride **C216**
 isobutenyl methyl ketone **M91**
 2-isobutoxynaphthalene **I94**
 isobutyl acetate **I87**
 isobutyl acrylate **I88**
 isobutyl adipate **D351**
 isobutyl alcohol **I85**
 isobutylamine **I89**
 isobutylcarbinol **M174**
 isobutylene **I86**
 2,4-D, isobutyl ester **D9**
 isobutylethylene **M284**
 isobutyl formate **I90**
p-isobutylhydratropic acid **I2**
 isobutyl iodide **I53**
 isobutyl isobutanoate **I91**
 isobutyl isobutyrate **I91**
 isobutyl ketone **D353**
 isobutyl methacrylate **I92**
 isobutyl α -methylacrylate **I92**
 isobutyl methyl carbinol **M281**
 isobutyl methyl ketone **M241**
 isobutylmethylemethanol **M281**
 isobutylmethylexanthine **I93**
 3-isobutyl-1-methylexanthine **I93**
 isobutyl 2-naphthyl ether **I94**
 2-(4-isobutylphenyl)propionic acid **I2**
 isobutyl phthalate **D354**
 isobutyl propanoate **I95**
 isobutyl 2-propenoate **I88**
 isobutyl propionate **I95**
 isobutyltrimethylethane **T314**
 isobutyl vinyl ether **I96**
 isobutyraldehyde **I97**
 isobutyric acid **I98**
 isobutyric acid, isobutyl ester **I91**
 isobutyric acid, methyl ester **M242**
 isobutyronitrile **I99**
 isocaramidine **D36**
 isochrysene **T336**
 isocornox **M40**
 isocrotonolactone **F124**
 isocrotyl chloride **C215**
 isocumene **P324**
 5-isocyanate-1-(isocyanatomethyl)-1,3,3-trimethylcyclohexane **I112**
 Isocyanate 390P **P114**
 isocyanatobenzene **P113**
 1-isocyanatobutane **B264**
 isocyanatoethane **E140**
 2-isocyanatoethyl methacrylate **M110**
 isocyanatomethane **M243**
 1-isocyanato-4-methylbenzene **T192**
 3-isocyanatomethyl-3,5,5-trimethylcyclohexylisocyanate
I112

isocyanatopropane **P333**
 1-isocyanatopropane **P333**
 isocyanic acid, butyl ester **B264**
 isocyanic acid, *o*-chlorophenyl ester **C246**
 isocyanic acid, *m*-chlorophenyl ether **C247**
 isocyanic acid, *p*-chlorophenyl ether **C248**
 isocyanic acid, 3,4-dichlorophenyl ester **D241**
 isocyanic acid, 3,3'-dimethoxy-4,4'-biphenylene ester **D379**
 isocyanic acid, hexamethylene ester **H55**
 isocyanic acid, methylenedi-4,1-cyclohexylene ester **M211**
 isocyanic acid, methylenedi-, 4-phenylene ester **M214**
 isocyanic acid, methyl ester **M243**
 isocyanic acid, methyl-*m*-phenylene ester **T175**
 isocyanic acid, 2-methyl-*m*-phenylene ester **T177**
 isocyanic acid, 1,5-naphthylene ester **N11**
 isocyanic acid, phenyl ester **P113**
 isocyanic acid, polymethylene polyphenylene ester **P114**
 isocyanic acid, propyl ester **P333**
 isocyanic acid, *p*-tolyl ester **T192**
 isocyanide **C481**
 isocyanuric acid **C491**
 isocyanuric chloride **T250**
 isocyanuric dichloride **D202**
 isocyclocitral **I100**
 isodiphenylbenzene **T29**
 isodrin **I101**
 isodurene **T88**
 isoeugenol **I102**
 isofedrol **E31**
 isofenphos **I103**
 isoflavone **I104**
 isoflavone, 4',7-dihydroxy- **D18**
 isoflavone, 4',5,7-trihydroxy- **G9**
 isofluorophate **I106**
 isoflurane **I105**
 isofluorophate **I106**
 Isofos **I103**
 isohexane **M273**
 isohexanol **M280**
 isohexyl alcohol **M280**
 isoindazole **I22**
 1*H*-isoindole-1,3(2*H*)-dione **P175**
 1*H*-isoindole-1,3(2*H*)-dione, 3a,4,7,7a-tetrahydro-2-[(1,1,2,2-tetrachloroethyl)thio]- **C58**
 1*H*-isoindole-1,3-(2*H*)-dione, 3a,4,7,7a-tetrahydro-2-[trichloromethyl]thio]- **C59**
 1,3-isoindolinedione **P175**
 isoinokosterone **E1**
 Isol **M275**
 isolan **I107**
 isolane **I107**
 D-isoleucine **I108**
 isomelamide **M47**
 isometasystox sulfone **D55**
 isomethylsystox **D54**
 isonaphthoic acid **N16**
 isonaphthol **N18**
 Isonex **I109**
 isoniazid **I109**
 isonicotinic acid hydrazide **I109**
 isonicotinic acid, 2-isopropylhydrazide, phosphate **I63**
 isonicotinitrile **C489**
 isonicotinoyl hydrazide **I109**
 isonitropropane **N139**
 isooctane **T314**
 isooctanol **M229**
 isooctaphenone **I110**
 isooctyl alcohol **M229**
 isooctyl 2,4-dichlorophenoxyacetate **D10**
 2(*or* 4)-isooctyl-4,6(*or* 2,6)-dinitrophenyl-2-butenolate **D505**
 2,4-D, isooctyl ester **D10**
 isopentanal **I140**
 isopentane **M172**
 isopentanol **M174**
 isopentene **M175**
 3-isopentenyl alcohol **M177**
 4-(2-isopentenyl)-1,2-diphenyl-3,5-pyrazolidinedione **F29**
 isopentyl acetate **I80**
 isopentyl alcohol **M174**
 isopentyl alcohol acetate **I80**
 isopentyl bromide **B179**
 isopentyl methyl ketone **M233**
 isopentyl nitrite **I81**
 isophenphos **I103**
 isophorone **I110**
 isophorone diamine **I111**
 isophorone diamine diisocyanate **I112**
 isophorone diisocyanate **I112**
 isophosphamide **I3**
 isophrin **P106**
 isophthalic acid **I113**
 isophthalonitrile **I114**
 isoprene **I115**
 isoprocarb **I116**
 isopropalin **I117**
 isopropanol **P297**
 isopropanolamine **A148**
 isopropene cyanide **M108**
 isopropenyl acetate **I118**
 isopropenylbenzene **M307**
 isopropenylcarbinol **M289**
 isopropenylethyl alcohol **M177**
 Isopropenyl methyl ketone **M179**
 isopropenyl nitrile **M108**
 2-isopropoxyethanol **I119**
 3'-isopropoxy-2-methylbenzanilide **M58**
 isopropoxymethylphosphoryl fluoride **S8**
 2-isopropoxyphenyl methylcarbamate **P315**
 2-isopropoxypropane **D359**
 3'-isopropoxy-*o*-toluanilide **M58**
 isopropyl acetate **I120**
 isopropylacetic acid **I141**

isopropylacetone **M241**
 isopropyl adipate **D357**
 isopropyl alcohol **P297**
 isopropyl aldehyde **I97**
 isopropylamine **I121**
 2-isopropylamino-4-methylamino-6-methylthio-1,3,5-triazine **D60**
 1-(isopropylamino)-3-(1-naphthoxy)-2-propanol **P321**
 4-isopropylbenzaldehyde **I122**
p-isopropylbenzaldehyde **I122**
 isopropylbenzene **C474**
 isopropylbenzene hydroperoxide **C475**
 isopropylbenzene peroxide **D264**
 3-isopropyl-(1*H*)-benzo-2,1,3-thiadiazin-4-one-2,2-dioxide **B38**
 3-isopropyl-2,1,3-benzothiadiazin-4-one-2,2-dioxide **B38**
 (R)-isopropyl *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)alaninate **F35**
 isopropyl borate **T298**
 isopropyl bromide **B186**
 isopropyl butanoate **I123**
 isopropyl butyrate **I123**
 2-[(*p*-isopropylcarbamoyl)benzyl]-1-methylhydrazine **P274**
N-4-isopropylcarbamoyl benzyl-*N'*-methylhydrazine hydrochloride **I1**
 isopropyl carbanilate **P305**
 isopropylcarbinol **I85**
 isopropyl cellosolve **I119**
 isopropyl chloride **C264**
 isopropyl 3-chlorocarbamate **C312**
 isopropyl chlorocarbonate **I124**
 isopropyl chloroformate **I124**
 isopropyl cyanide **I99**
 isopropylcyclohexane **I125**
 isopropyl 4,4'-dichlorobenzilate **C276**
 isopropyl 3,4-diethoxycarbanilate **D283**
 isopropyl *N*-(3,4-diethoxyphenyl)carbamate **D283**
 isopropyl dimethyl carbinol **M277**
 4-isopropyl-2,6-dinitro-*N,N*-dipropylaniline **I117**
 isopropylene glycol **P327**
 isopropylene nitrate **P329**
 isopropyl ether **D359**
 isopropylethylene **M175**
 isopropyl ethyl ether **E83**
 isopropyl fluophosphate **I106**
 isopropylformaldehyde **I97**
 isopropyl formate **I126**
 isopropylformic acid **I98**
 isopropyl glycidyl ether **G30**
 isopropyl glycol **I119**
 isopropylidene acetone **M91**
 2-isopropylideneamino-oxyethyl (R)-2-[4-(6-chloroquinoxalin-2-yloxy)phenoxy]propionate **P299**
 4,4'-isopropylidenebis(2,6-dibromophenol) **T39**
 4,4'-isopropylidenediphenol **B133**
 4,4'-isopropylidenediphenol diglycidyl ether **B134**
 isopropylidene glycerol **S101**
 1,2-isopropylideneglycerol **S101**
 2,3-isopropylideneglycerol **S101**
 4-isopropylidene-1-methylcyclohexane **T37**
 isopropyl ketone **D447**
N-isopropylmaleimide **I127**
 isopropyl (*E,E*)-(R*S*)-11-methoxy-3,7,11-trimethyldodeca-2,4-dienoate **M127**
N-isopropyl-1 α -(2-methylazo)-*p*-toluamide **A272**
 1-isopropyl-4-methyl-1,3-cyclohexadiene **T34**
 1-isopropyl-4-methylcyclohexane **M51**
 2-isopropyl-5-methylcyclohexanol **M53**
 1-isopropyl-2-methylethylene **M285**
N-isopropyl- α -(2-methylhydrazino)-*p*-toluamide **P274**
N-isopropyl- α -(2-methylhydrazino)-*p*-toluamide monohydrochloride **I1**
 isopropyl methyl ketone **M244**
*N*2-isopropyl-*N*4-methyl-6-methylthio-1,3,5-triazine-2,4-diamine **D60**
 2-(4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl)nicotinic acid **I6**
 3-isopropyl-5-methylphenyl methylcarbamate **P286**
 isopropyl methylphosphofluoridate **S8**
 isopropyl methylphosphonofluoridate **S8**
 1-isopropyl-3-methyl-5-pyrazolyl dimethylcarbamate **I107**
 2-isopropyl-naphthalene **I128**
 β -isopropyl-naphthalene **I128**
 isopropyl nitrate **I129**
 isopropyl nitrile **I99**
p-isopropyl-nitrobenzene **N109**
 2-isopropyl-4-pentenamide **A86**
 isopropyl peroxydicarbonate **D360**
 4-isopropylphenol **I130**
p-isopropylphenol **I130**
 3-isopropylphenol methylcarbamate **I131**
m-isopropylphenol methylcarbamate **I131**
 isopropyl phenylcarbamate **P305**
 3-(4-isopropylphenyl)-1,1-dimethylurea **I133**
 2-isopropylphenyl methylcarbamate **I116**
 3-isopropylphenyl methylcarbamate **I131**
 isopropylphenyl urethane **P305**
 isopropyl phosphoramidic acid ethyl 4-(methylthio)-*m*-tolyl ester **F3**
 isopropyl phosphorofluoridate **I106**
 1-isopropylpropanol **M278**
 isopropyltoluene **C537**
 2-isopropyltoluene **C539**
 3-isopropyltoluene **C538**
 α -isopropyl- α -[*p*-(trifluoromethoxy)phenyl]-5-pyrimidinemethanol **F89**
 isopropylxanthic acid, sodium salt **P343**
 isoprothiolane **I132**
 isoproturon **I133**
 isopseudocumenol **T320**
 isopulegol **I134**
 isopurine **P346**

isoquinoline **I135**
 isosafrole **I136**
 isosafrole *n*-octylsulfoxide **S148**
 isoselenourea **S21**
 isosorbide **I137**
 isosystox sulfone **D56**
 3(2*H*)-isothiazolone, 5-chloro-2-methyl- **C212**
 isothiocyanatobenzene **P115**
 isothiocyanatomethane **M245**
 3-isothiocyanato-1-propene **A87**
 isothiocyanic acid, phenethyl ester **P70**
 isothiocyanic acid, *p*-phenylene ester **B138**
 isothiocyanic acid, phenyl ester **P115**
 isothiosemicarbazide **T144**
 isothiurea **T146**
 Isotol **M28**
 isotretinoin **I138**
 Isotron 11 **F78**
 isourea **U12**
 isouron **I139**
 isovaleraldehyde **I140**
 isovaleric acid **I141**
 isovaleric acid, allyl ester **A88**
 isovaleric acid, butyl ester **B265**
 isovaleric acid, methyl ester **M246**
 isovaleric aldehyde **I140**
 isovalerone **D353**
 isovaleronitrile **I142**
N-isovaleryl-L-valyl-L-valyl-3-hydroxy-6-methyl- γ -
 aminoheptanoyl-L-alanyl-3-hydroxy-6-methyl- γ -
 aminoheptanoic acid **P50**
 isoxanthine **X2**
 isoxathion **I143**
 Isoxyl **I139**
 Istin **C350**
 isuron **I139**
 IT3233 **F85**
 itaconic acid **I144**
 Italcementi **C99**
 ITC **P286**
 Ivalor **P234**
 Jaguar **G51**
 Janimine **I15**
 Japan agar **A58**
 Japan isinglass **A58**
 Japan red 204 **D27**
 Japan Red No. 103 **E29**
 Japan Yellow **Q10**
 Japan yellow 201 **F51**
 jasad **Z2**
 jasmoline I **J1**
 jasmolin I **J1**
 jasmolin II **J2**
 jasmone **J3**
cis-jasmone **J3**
 jasper **S29**
 Jatropur **T203**

Jayflex DHP **D341**
 Jayflex DIDP **D355**
 Jayflex DOA **D513**
 Jayflex DTDP **D577**
 Jeffosol DM **M135**
 Jestryl **C60**
 jet fuel **K7**
 Jodcyan **C485**
 jodfenphos **I50**
 Jubilee **M328**
 Judgan pitch **A249**
 K-17 **T99**
 K1441 **M209**
 Kabre **D511**
 Kabrol **D511**
 kadethrin **K1**
 Kaiod **P256**
 Kalgan **P64**
 kalinite **A105**
 kalium **P237**
 Kalium-Duriles **P243**
 Kalmin **P58**
 Kalpur TE **H51**
 kampstaff Lost **M359**
 Kanechlor 500 **P220**
 Kanepar **C124**
 Kaochlor **P243**
 kaolin **K2**
 karamate **M19**
 karaya gum **K3**
 Karbaril **C63**
 Karbromal **C85**
 karbutilate **K4**
 Karion **S104**
 Karmex **D579**
 Karmex Monuron Herbicide **M350**
 Karmex W. monuron herbicide **M350**
 Karphos **I143**
 Kasser **D536**
 kasugamycin **K5**
 Kasumin **K5**
 Katalon **D560**
 Kathon **O19**
 Kathon CG **C212**
 katilo gum **K3**
 Katron **W1**
 Kayaku Blue B Base **D95**
 Kayametone **M145**
 Kayanex **M215**
 Kayaphos **P298**
 Kay Ciel **P243**
 Kayvalerate **F28**
 KCO-3001 **F15**
 Keetak **F20**
 Keflex **C100**
 Keical-Ace **C43**
 Kelaran **P300**

kelevan **K6**
 Kemikar **C84**
 Kemiron **E72**
 Kemsol **S92**
 Kenofuran **C68**
 Kepone **C119**
 Keramin **D316**
 kerb **P339**
 kerosene **K7**
 kerosine **K7**
 ketene **K8**
 ketine **D452**
 Ketjensept **C113**
 ketoconazole **K9**
 ketocyclopentane **C525**
 17 β -(1-ketoethyl)- Δ^5 -androsen-3 β -ol **P270**
 ketohexamethylene **C509**
 2-ketohexamethyleneimine **C55**
 ketohydroxyestrin **E53**
 ketole **I31**
 γ -keto- β -methoxy- δ -methylene- $\Delta\alpha$ -hexenoic acid **P21**
 ketopentamethylene **C525**
 ketoprofen **K10**
 β -ketopropane **A17**
 α -ketopropionic acid **P368**
 L-3-ketothreohexuronic acid lactone **A248**
 4-ketovaleric acid **L40**
 Kevadon **T99**
 Khinaldin **Q4**
 Kicker **P354**
 Kidan **I62**
 Kieselguhr **D97**
 Killex **T68**
 Kilumal **F18**
 Kilval **V9**
 kinetin **K11**
 King Chlor **S74**
 Kings gold **A245**
 Kiros **B109**
 Kisvax **C84**
 Kitazin L **I61**
 Klartan **F94**
 Klerat **B150**
 Kloben **N32**
 Knollide **P256**
 Koban **E185**
 Kodaflex DIBP **D354**
 Kodaflex DIDP **D355**
 Kodaflex DMP **D450**
 Kodaflex DOA **D513**
 Kodaflex TXIB **T316**
 Kodalfex DOP **D519**
 Kombetin **O40**
 Konesta **T226**
 Korforn 22 **C192**
 Korlan **F8**
 KP 140 **T348**
 Kraft lignin **L42**
 Krenite **F107**
 Krumkil **F116**
 kryolith **C472**
 Kumadu **W1**
 Kumatox **W1**
 Kuran **F14**
 Kusgard **A71**
 Kwell's **H123**
 Kyanol **A209**
 Kyowaad 1000 **H108**
 Lacovyl **P235**
 Lacquer Orange V **O27**
 lactamide, *N*-ethylcarbanilate (ester), D- **C66**
 Lactarin **C91**
 lactic acid **L1**
 Lactobene **R12**
 Lactoflavine **R12**
 lactonitrile **L2**
 lactonitrile, 2-methyl- **A18**
 lactose, β **L3**
 β -lactose **L3**
 β -D-lactose **L3**
 Laevosan **F111**
 Laevuflex **F111**
 laevulose **F111**
 Laivin **C63**
 Lake Blue B Base **D95**
 lake red CBA **D27**
 Lambrol **F44**
 Lame gum **K3**
 Lamoryl **G46**
 lamp black **C73**
 Lanacard **D339**
 Lanacordin **D339**
 Lance **C356**
 Landisan **M137**
 Landomycin **O29**
 Lanette 16 **C102**
 lannate **M126**
 lanthanum **L4**
 lanthanum chloride (La₂Cl₆) **L5**
 lanthanum chloride (LaCl₃) **L5**
 lanthanum trichloride **L5**
 Largactil (as hydrochloride) **C310**
 Larvadex **C545**
 Larvin **T128**
 lasiocarpine **L6**
 Lasix **F112**
 latex **P222**
 laughing gas **N183**
 Laundrosil **B39**
 lauraldehyde **D584**
 lauramide DEA **L7**
 lauric acid **L8**
 lauric acid diethanolamide **L7**
 lauridiethanolamide **L7**

Laurostearic acid **L8**
 Laurox Q **L9**
 lauroyl diethanolamide **L7**
 (lauroyloxy)tributylstannane **T217**
 lauroyl peroxide **L9**
 laurydol **L9**
 lauryl alcohol **D588**
 lauryl aldehyde **D584**
 laurylbenzenesulfonic acid **D589**
 laurylguanidine acetate **D594**
 lauryl mercaptan **D586**
 laurylpyridinium chloride **L10**
 lauryl trimethylammonium bromide **D592**
 LCR **V24**
 LCR-sulfate **V25**
 LDPE **P224**
 LE 29060 **V21**
 29060-LE **V20**
 lead **L11**
 lead acetate **L12**
 lead(IV) acetate **L32**
 lead acetate, basic **L29**
 lead arsenate **L13**
 lead arsenite **L14**
 lead, bis(acetato-O)tetrahydroxytri- **L29**
 lead, bis(dimethylcarbamodithioato-S,S')-, (T-4)- **L18**
 lead bis(thiocyanate) **L33**
 lead boron fluoride **L21**
 Lead Bottoms **L30**
 lead chloride **L15**
 lead chloride (PbCl₂) **L15**
 lead chromate **L16**
 lead chromium oxide **L16**
 lead cyanide **L17**
 lead dichloride **L15**
 lead difluoride **L22**
 lead diiodide **L24**
 lead dimethyldithiocarbamate **L18**
 lead dinitrate **L25**
 lead dioxide **L19**
 lead diperchlorate **L26**
 lead diphosphate **L27**
 lead distearate **L20**
 lead dithiocyanate **L33**
 lead flake **L11**
 lead fluoborate **L21**
 lead fluoride **L22**
 lead fluorosilicate **L23**
 lead hexafluorosilicate **L23**
 lead hydrogen arsenate **L13**
 lead iodide **L24**
 lead methanoate **L12**
 lead nitrate **L25**
 lead orthophosphate **L27**
 lead oxide brown **L19**
 lead oxide phosphonate **L28**
 lead perchlorate **L26**
 lead peroxide **L19**
 lead phosphate **L27**
 lead phosphite dibasic **L28**
 lead silicon fluoride **L23**
 lead stearate **L20**
 lead subacetate **L29**
 lead sulfate **L30**
 lead sulfide **L31**
 lead sulfocyanate **L33**
 lead superoxide **L19**
 lead tetraacetate **L32**
 lead tetraethyl **T66**
 lead tetrafluoroborate **L21**
 lead tetramethyl **T90**
 lead thiocyanate **L33**
 leaf alcohol **H74**
 Lebaycid **F24**
 Ledate **L18**
 Leecure B Series **B147**
 Legurame **C66**
 LeIF **I39**
 Lemax **P130**
 Lemonol **G12**
 lenacil **L34**
 Lenamon **L34**
 Lenoxin **D339**
 Lentagran **P356**
 Lentin **C60**
 4-lepidin **M299**
 lepidine **M299**
 Lepinal **P79**
 leptophos **L35**
 Leptox **C128**
 Lerbek **C363**
 Lermol **C364**
 Leropropoxyphene **L39**
 Le san **F2**
 leucethane **U13**
 leucine **L36**
 DL-leucine **L36**
 Leucobasal **M144**
 leucoharmin **H7**
 leucoline **I135**
 leucoline **Q9**
 leukaemomycin C **D23**
 Leukeran **C111**
 Leukerin **M63**
 leukocyte interferon **I39**
 Leukol **Q9**
 leurocristine **V24**
 leurocristine sulfate (1:1) **V25**
 levodopa **L37**
 levofalan **M49**
 levonorgestrel **L38**
 levopropoxyphene **L39**
 Levothyroxine **T156**
 Levoxin **H87**

levulic acid **L40**
 levulinic acid **L40**
 levulose **F111**
 Lewisite **L41**
 Lexguard B **B269**
 Liafos **P350**
 Libavium fuming spirit **T160**
 lichemic acid **F115**
 Lidocaine **L43**
 Light Green N **M9**
 light ligroin **N5**
 Lignasan **E144**
 lignin alkali **L42**
 lignocaine **L43**
 lilial **L44**
 Lilly 53838 **F13**
 Lilyal **L44**
 Limbux **C33**
 lime **C37**
 lime chloride **C34**
 lime-nitrogen **C29**
 limestone **C25**
 lime sulfur **C42**
 Limil **C33**
 limonene **L45**
 (+)-limonene **L46**
 α-limonene **L45**
 D-limonene **L46**
 (R)-limonene **L46**
 (R)-(+)-limonene **L46**
 limonene oxide **C343**
 Limstab **L30**
 linalol **L47**
 linalool **L47**
 linalyl alcohol **L47**
 lindane **H10**
 ε-lindane **L48**
 Lindol **T361**
 Linex 4L **L50**
 Linodil **I38**
 linoleic acid **L49**
 linolic acid **L49**
 Lintex **N52**
 linuron **L50**
 Lion **C99**
 Liozan **H87**
 Lipamid **C358**
 liparite **F80**
 lipase **L51**
 Lipol L8 **O13**
 Lipopill **P88**
 Liposorb S-20 **P229**
 Lipozyme **L51**
 Liquamycin **O64**
 liquefied petroleum gas **L59**
 liquid bright platinum **P212**
 Liquid Lightning **S137**
 liquid pitch oil **C453**
 Liromat **M10**
 Liromort **D510**
 Lironion **D324**
 Lirostanol **F25**
 Lissamine Green B **C389**
 lithic acid **U14**
 lithium **L52**
 lithium alanate **L53**
 lithium aluminium hydride **L53**
 lithium aluminohydride **L53**
 lithium chloride oxide **L55**
 lithium hydride **L54**
 lithium hypochlorite **L55**
 lithium monohydride **L54**
 lithium oxychloride **L55**
 lithocholic acid **L56**
 lithographic stone **C25**
 Lithosol Deep Blue B **I25**
 Lithosol Scarlet Base M **M261**
 locust bean gum **L57**
 Lo-estrin **N207**
 Logic **F17**
 Lomudal **S57**
 lomustine **L58**
 Lontrel **C364**
 Lontryx **C364**
 Lopress **H85**
 Loralan-CH **C324**
 Lorate **M328**
 Lorix **B187**
 Lormin **C139**
 Lorotheidol **T122**
 Lotrimin **C365**
 Loturine **H6**
 Lovozal **F5**
 Loweserp **R3**
 LPG **L59**
 LPK **V40**
 LS4442 **T340**
 Lubestine **T3**
 Lucarotin 10% Feed **C89**
 Lullamin **M117**
 Lumbial **O48**
 Lumbrical **P200**
 Luminous **P226**
 Lumosaure A **D589**
 Luperco **D264**
 Luperox **D264**
 Lupersol **M222**
 lupinidine **S105**
 lupogum **L57**
 Lustra **K2**
 luteal hormone **P282**
 lutecium **L60**
 luteine **P282**
 lutetium **L60**

2,3-lutidine **L61**
 2,4-lutidine **L62**
 2,5-lutidine **L63**
 2,6-lutidine **L64**
 α,α' -lutidine **L64**
 β -lutidine **E167**
 Lutinyl **C139**
 Luvomag **M6**
 Luxan Alzodef **C479**
 Luxan Teceal **C108**
 lycopene **L65**
 lycopene, *all-trans*- **L65**
 lycopene 7 **L65**
trans-lycopene **L65**
 Lyder **F28**
 Lye **P254**
 lymecycline **L66**
 lymphoblastoid interferon **I39**
 lynestrenol **L67**
 LYP 97 **L9**
 L-lysine, N⁶-[[[4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-2-naphthacenyl]carbonyl]amino]methyl]-, [4S-(4 α ,4a α ,5a α ,6 β ,12a α)]- **L66**
 lyxose, D- **L68**
 α -D-lyxose **L68**
 D-lyxose **L68**
 M 1586 **C490**
 M2452 **D569**
 M34 **M27**
 M3432 **T162**
 1-N-2-MA **M264**
 MAAC **H77**
 MACE **C148**
 Machal **X4**
 Machete **B196**
 Mackernium CTC-30 **C105**
 Macquer's salt **P238**
 Macrochantin **N115**
 Macrogol **P225**
 Magenta I **M1**
 mageon **Q8**
 Magic Methyl **M224**
 Magister **F6**
 Maglite **M6**
 magnesa preprata **M6**
 magnesium arsenate **M2**
 magnesium chlorate **M3**
 magnesium dichlorate **M3**
 magnesium dinitrate **M5**
 magnesium diperchlorate **M7**
 magnesium fluorosilicate **M4**
 magnesium hexafluorosilicate **M4**
 magnesium monoxide **M6**
 magnesium nitrate **M5**
 magnesium oxide **M6**
 magnesium perchlorate **M7**
 magnesium phosphide **M8**
 magnesium silicofluoride **M4**
 magniosan **M5**
 Magox **M6**
 magron **M3**
 Magus **F6**
 Major components are polychloro-2-[chloromethyl-sulfonamido]diphenyl ethers (PCSDs) **E188**
 Malachite Green **M9**
 Malachite Green chloride **M9**
 Malachite Green G **C400**
 malaaxon **M10**
 malathion **M11**
 malathion-O-analog **M10**
 Malehid **M14**
 maleic acid **M12**
 maleic anhydride **M13**
 maleic hydrazide **M14**
 maleinic acid **M12**
 malenic acid **M12**
 Malepin **M14**
 malestrone **T38**
 malic acid **M15**
 malic acid hydrazide **M14**
 Malice **B37**
 Mallard **F19**
 Mallorol **T143**
 malonaldehyde **M16**
 malondialdehyde **M16**
 malonic acid **M17**
 malonic acid dinitrile **M18**
 malonic acid, ethyl ester nitrile **E110**
 malonic acid, thallium salt **T105**
 malonic aldehyde **M16**
 malonic dialdehyde **M16**
 malononitrile **M18**
 Maloran **C116**
 Malzid **M14**
 MAM **M159**
 MAM acetate **M160**
 mancozeb **M19**
 DL-mandelic acid **M20**
 (\pm)-mandelic acid **M20**
 mandelic acid, 3,3,5-trimethylcyclohexyl ester **C496**
 maneb **M21**
 manganese **M22**
 manganese binoxide **M24**
 manganese cyclopentadienyl tricarbonyl **M23**
 manganese dinitrate **M26**
 manganese dioxide **M24**
 manganese ethylenebis(dithiocarbamate) **M21**
 manganese 2-methylcyclopentadienyl tricarbonyl **M25**
 manganese nitrate **M26**
 manganese oxide **M24**
 manganese oxide **M27**
 manganese(IV) oxide **M24**
 manganese oxide (Mn₃O₄) **M27**

manganese potassium oxide **P260**
 manganese tetroxide **M27**
 manganese, tricarbonyl(methyl- π -cyclopentadienyl)- **M25**
 manganese, tricarbonyl[(1,2,3,4,5- π)-1-methyl-2,4-cyclopentadien-1-yl]- **M25**
 Manhao **F21**
 Manipulator **C141**
 manna sugar **M28**
 marnistol **M28**
 Mannit **M28**
 mannitol **M28**
 D-mannitol **M28**
 mannitol mustard **M29**
 mannomustine (dihydrochloride) **M29**
 mannomustine hydrochloride **M29**
 mannose **M30**
 D-mannose **M30**
 D-(+)-mannose **M30**
 Mantis **P306**
 Manzate **M21**
 manzeb **M19**
 MAOH **M281**
 maple lactone **M31**
 Maprofix WAC **S76**
 Marailid phosphate **I63**
 marble **C25**
 Marezine **C497**
 Marfotoks **M37**
 Margosan-O **A258**
 Marisan **D260**
 Marlon A **S65**
 Marrel P **D536**
 Marshal **C83**
 marsh gas **M112**
 Masoten **T225**
 Master **T250**
 Match **C480**
 Matikus **B150**
 Matin **I133**
 Mator **H106**
 Matromycin **O29**
 Mauguinite **C484**
 Mavrik **F94**
 Maxforce **H86**
 2-maythic acid **N16**
 MB-6046 **P215**
 MBAO **M39**
 MBCP **L35**
 MBK **H67**
 MBR 12325 **M43**
 MBR 8251 **P54**
 4-MBSA **T178**
 MBT **M61**
 20-MC **M190**
 3-MC **M190**
 MCCI Carbide **C24**
 MCF **M188**

MCN-485 **Z25**
 MCN 1025 **N201**
 MCPA **M32**
 MCPA-thioethyl **M33**
 MCPB **M34**
 MCPP **M40**
 MCT **M23**
 MDA **M218**
 MDBA **D165**
 MDEA **M206**
 MDI **M214**
 2-ME **M62**
 Meadol MRM **L42**
 meat sugar **I37**
 MEB **M21**
 meballymal **Q3**
 Mebazine **A252**
 mebeverine **M35**
 mebhdyrolin **M36**
 mecarbam **M37**
 mechlorethamine **M38**
 mechlorethamine oxide **M39**
 mechlorethamine N-oxide **M39**
 mecoprop **M40**
 mecrylate **M196**
 Mediflor FC 43 **P55**
 Medihaler Ergotamine **E44**
 Medomet **M208**
 Medrin **T134**
 Meen **A258**
 Mefacit **M42**
 mefenacet **M41**
 Mefenal **S133**
 mefenamic acid **M42**
 mefluidide **M43**
 Megace **M44**
 Megatox **F53**
 Megestat **M44**
 megestrol acetate **M44**
 Meguan **M100**
 Mehltaumittel **D593**
 Meiji Herbiace **B110**
 MeIQ **M45**
 MeIQx **M46**
 MEK **M220**
 ME-6K **M140**
 MEK oxime **M221**
 MEK peroxide **M222**
 Meladinine **M129**
 melamine **M47**
 melatonin **M48**
 melinite **P187**
 melipan **N2**
 Melitoxin **D262**
 melkeb **D375**
 Mellaril **T143**
 Mellerette **T143**

Mellinese **C311**
 Mellite 310 **T339**
 Meloxine **M129**
 melphalan **M49**
 Melsed **M119**
 Meltatox **D593**
 Mema **M137**
 menazon **M50**
 mendrin **E25**
 Menformon A **E53**
 Menophase **M92**
 Menorest **E50**
 menstranol-norethynodrel mixture **E28**
 menthacampfor **M54**
p-mentha-1,3-diene **T34**
p-mentha-1,4(8)-diene **T37**
p-mentha-1,8-diene **L45**
 (S)-(+)-*p*-mentha-6,8,-dien-2-one **C93**
trans-*p*-menthane **M51**
 (1*RS*,4*RS*)-*p*-menthane-1,8-diol **T33**
cis-*p*-menthane-1,8-diol **T33**
p-menthane-1,8-diol **T32**
p-menthane hydroperoxide **M52**
p-menthan-3-ol **M53**
 (1*R*,3*R*,4*S*)-(-)-*p*-menth-8-en-3-ol **I134**
p-menth-1-en-8-ol **T36**
p-menth-1-en-8-ol **T35**
 menthol **M53**
 menthol **M54**
 DL-menthol **M54**
 (±)-menthol **M54**
 (±)-*cis*-1,3-*trans*-1,4-menthol **M54**
 menthomenthol **M54**
 menthyl alcohol **M53**
p-menth-8-yl hydroperoxide **M52**
 Meobal **X16**
 Meothrin **F18**
 MEP **F11**
 MEP **E163**
 mepacrine **M55**
 mephenamic acid **M42**
 mephosfolan **M56**
 meprobamate **M57**
 mepronil **M58**
 Meprospam **M57**
 Mequin **M119**
 Mequinol **M144**
 Meractinomycin **A46**
 Meralluride **S77**
 Meranol **G12**
 mercaptazole **M122**
 mercaptoacetic acid **M59**
 mercaptoacetic acid, methyl ester **M248**
 (mercaptoacetyl)methylcarbamic acid, ethyl ester, *S*-ester
 with *O,O*-diethyl phosphorodithioate **M37**
 2-mercaptobenzimidazole **M60**
 2-mercaptobenzothiazole **M61**
 mercaptobenzothiazole disulfide **D572**
 mercaptobenzthiazyl ether **D572**
 mercaptodiacetic acid **T130**
 Mercaptodimethur **M123**
 1-mercaptododecane **D586**
 2-mercaptoethanoic acid **M59**
 2-mercaptoethanol **M62**
 2-mercapto-4-hydroxy-6-*n*-propylpyrimidine **P337**
 mercaptomethane **M115**
 2-mercapto-1-methylimidazole **M122**
 1-mercaptooctadecane **O3**
 1-mercaptooctane **O10**
 Mercaptophos **F24**
 α-mercaptopropanoic acid **T132**
 2-mercaptopropionic acid **T132**
 α-mercaptopropionic acid **T132**
 2-mercapto-6-propyl-4-pyrimidone **P337**
 6-mercaptopurine **M63**
 mercaptosuccinic acid diethyl ester, *S*-ester with *O,O*-
 dimethyl phosphorodithioate **M11**
 mercaptothion **M11**
 Mercardan **S77**
 Mercazolyl **M122**
 Mercuhydrin **S77**
 Mercuran **M137**
 mercurate(1-), ethyl[2-mercaptobenzoato(2-)-*O,S*]-, sodium
 salt **T133**
 mercurate(2-), [orthoborato(3-)-*O*]phenyl-, dihydrogen
P117
 mercurialin **M154**
 mercuric benzoate **M67**
 mercuric bromide **M69**
 mercuric cyanide **M72**
 mercuric diacetate **M65**
 mercuric iodide **M76**
 mercuric nitrate **M78**
 mercuric oxide red **M82**
 mercuric oxide yellow **M82**
 mercuric oxycyanide **M83**
 mercuric potassium iodide **P266**
 mercuric salicylate **M84**
 mercuric sulfate **M86**
 mercuric sulfocyanate **M87**
 mercuric sulfocyanide **M87**
 mercuric thiocyanate **M87**
 mercurisalicyclic acid **M84**
 mercuriol **M79**
 mercurothiolate **T133**
 mercurous bromide **M68**
 mercurous chloride **M70**
 mercurous chloride **C47**
 mercurous gluconate **M74**
 mercurous iodide **M75**
 mercurous nitrate **M77**
 mercurous sulfate **M85**
 mercury **M64**
 mercury(II) acetate **M65**

mercury, (acetato-*O*)phenyl- **P116**
 mercury amide chloride **M66**
 mercury ammonium chloride **M66**
 mercury benzoate **M67**
 mercury bichloride **M71**
 mercury biniodide **M76**
 mercury(I) bromide **M68**
 mercury(II) bromide **M69**
 mercury chloride **M71**
 mercury(I) chloride **M70**
 mercury I chloride **C47**
 mercury(II) chloride **M71**
 mercury(II) cyanide **M72**
 mercury cyanide oxide **M83**
 mercury, diethyl- **D308**
 mercury dithiocyanate **M87**
 mercury, ethyl (hydrogen *o*-mercaptobenzoato)-, sodium salt **T133**
 mercury fulminate **M73**
 mercury gluconate **M74**
 mercury(I) iodide **M75**
 mercury(II) iodide **M76**
 mercury acetate **M65**
 mercury(1+), methyl- **M249**
 mercury monochloride **M70**
 mercury(I) nitrate **M77**
 mercury(II) nitrate **M78**
 mercury nucleate **M79**
 mercury oleate **M80**
 mercury(I) oxide **M81**
 mercury(II) oxide **M82**
 mercury oxycyanide **M83**
 mercury perchloride **M71**
 mercury pernitrate **M78**
 mercury potassium iodide **P266**
 mercury protoiodide **M75**
 mercury protonitrate **M77**
 mercury salicylate **M84**
 mercury subchloride **C47**
 mercury(I) sulfate **M85**
 mercury(II) sulfate **M86**
 mercury(II) thiocyanate **M87**
 Merfen **P117**
 Merfen-styli **P120**
 Merit **I8**
 Merkon **P154**
 Merocets **C104**
 Merpafol **C58**
 Merpan **C59**
 merphalan **M88**
 merphos **M89**
 merrilite **Z2**
 Merseptyl **T133**
 Mersolite 1 **P119**
 Mersolite 2 **P118**
 mesidine **T305**
 mesitol **T322**
 mesityl alcohol **T322**
 mesitylamine **T305**
 mesitylene **M90**
 mesityl oxide **M91**
 Mesodrin **O57**
 mesoinosite **I37**
 Mesonex **I38**
 mestranol **M92**
 Mesurol **M123**
 Mesurol phenol **M123**
 3-mesitylbutanone-*O*-methylcarbamoyloxime **B225**
 mesyl fluoride **M114**
 Metab-Auxil **P35**
 Metabolite I **O63**
 Metacar **H80**
 metacetaldehyde **M94**
 metacetic acid **P310**
 Metacide **P14**
 Metacil **M312**
 Metacil **A123**
 metadelphene **D319**
 metalaxyl **M93**
 metaldehyde **M94**
 metallic arsenic **A240**
 metallic tin **T158**
 metalum problematum **T16**
 metamitron **M95**
 Metamitrone **M95**
 metam-sodium **M96**
 metanilic acid **M97**
 metaoxedrin **P106**
 metaphos **P14**
 metaphosphoric acid ($\text{H}_6\text{P}_6\text{O}_{18}$) hexasodium salt **S69**
 metaproterenol **O33**
 metasymptol **P106**
 metasynephrine **P106**
 Metasystemox R **O57**
 Metasystox R **O57**
 Metaxanin **M93**
 metazachlor **M98**
 metepa **M99**
 metformin HCl **M100**
 metformin hydrochloride **M100**
 methabenzthiazuron **M101**
 methacon **M118**
 methacrifos **M102**
 methacrolein **M103**
 methacrolein diacetate **M104**
 methacroyl anhydride **M107**
 methacrylaldehyde **M103**
 methacrylamide **M105**
 methacrylic acid **M106**
 α -methacrylic acid **M106**
 methacrylic acid amide **M105**
 methacrylic acid, butyl ester **B267**
 methacrylic acid, 2-hydroxypropyl ester **H117**
 methacrylic acid, isobutyl ester **I92**

methacrylic acid, methyl ester **M252**
 methacrylic anhydride **M107**
 methacrylic chloride **M109**
 methacrylonitrile **M108**
 α -methacrylonitrile **M108**
 methacryloyl chloride **M109**
 methacryloyloxyethyl isocyanate **M110**
 methallyl alcohol **M289**
 methallylcarbinol **M177**
 methallyl chloride **C216**
 2-methallyl chloride **C216**
 α -methallyl chloride **C178**
 β -methallyl chloride **C216**
 γ -methallyl chloride **C176**
 methallylidene diacetate **M104**
 methamidophos **M111**
 methaminodiazepoxide **C120**
 metham sodium **M96**
 methanal **F100**
 methanamide **F101**
 methanamine **M154**
 methane **M112**
 methanearsonic acid disodium salt **D601**
 methanecarbothiolic acid **T116**
 methane carboxamide **A10**
 methanecarboxylic acid **A12**
 methane, chloromethoxy- **C214**
 methanedicarboxylic acid **M17**
 methanesulfonic acid **M113**
 methanesulfonic acid, methyl ester **M253**
 methanesulfonyl fluoride **M114**
 methanetetramethylol **P35**
N,N'-methanetetraylbis(cyclohexanamine) **D267**
 methanethiol **M115**
 methane trichloride **C201**
 methanium hydroxide **T86**
 6,9-methano-2,4,3-benzodioxathiepin 3,3-dioxide **E21**
 6,9-methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3 α ,5 α ,6 β ,9 β ,9 α)- **E20**
 methanoic acid **F104**
 4,7-methano-1*H*-indene, 1,2,3,4,5,6,7,8,8-nonachloro-2,3,3a,4,7,7a-hexahydro-, (1 α ,2 β ,3 α ,3 α ,4 β ,7 β ,7 α)- **N190**
 methanol **M116**
N-methanolacrylamide **H113**
 methanon **M203**
 Methaphos **M111**
 methapyrapone **M329**
 methapyrilene **M117**
 methapyrilene hydrochloride **M118**
 methaqualone **M119**
 methazole **M120**
 methenamine **H57**
 1,3,4-metheno-1*H*-cyclobuta[*cd*]pentalene-2-pentanoic acid, 1,1a,3,3a,4,5,5a,5b,6-decachlorooctahydro-2-hydroxy- γ -oxo-, ethyl ester **K6**
 methenylaldehyde **M103**
 methenyl trichloride **C201**
 Methiacil **M312**
 methiamitron **M95**
 methibenzuron **M101**
 methidathion **M121**
 methimazole **M122**
 methiocarb **M123**
 D-methionine **M124**
 (*R*)-(-)-methionine **M124**
 methocarbamol **M125**
 Methocel A **M185**
 Methocel MC **M185**
 methomyl **M126**
 methoprene **M127**
 α -methopterin **M128**
 methotrexate **M128**
 Methoxone **M32**
 methoxsalen **M129**
 methoxtriglycol **T283**
 methoxyacetic acid **M130**
 2-methoxyacetic acid **M130**
 methoxyacetone **M131**
 1-methoxyacetone **M131**
 methoxyaniline **A215**
 2-methoxyaniline **A213**
m-methoxyaniline **A214**
o-methoxyaniline **A213**
 2-methoxy-*p*-anisidine hydrochloride **D378**
 4-methoxy-*o*-anisidine hydrochloride **D378**
 2-methoxyanisole **V18**
 2-methoxybenzenamine **A213**
 3-methoxybenzenamine **A214**
 4-methoxybenzenamine **A215**
 4-methoxy-1,3-benzenamine **D73**
 methoxybenzene **A216**
 4-methoxy-1,3-benzenediamine sulfate **D74**
 7-methoxy-2*H*-1-benzopyran-2-one **M133**
 4-methoxybenzoyl chloride **A217**
p-methoxybenzoyl chloride **A217**
 2-methoxy-4,6-bis(isopropylamino)-s-triazine **P288**
 methoxycarbonyl chloride **M188**
 methoxycarbonylethylene **M153**
 2-methoxycarbonyl-1-methylvinyl dimethyl phosphate **M330**
 (*E*)-*O*-2-methoxycarbonylprop-1-enyl *O,O*-dimethyl phosphorothioate **M102**
 methoxycellulose **M185**
 methoxychlor **M132**
 (8 α ,6*R*)-6'-methoxycinchonine **Q6**
 7-methoxycoumarin **M133**
 2-methoxy-3,6-dichlorobenzoic acid **D165**
 methoxydiglycol **M135**
 5-methoxy-2-[(dimethoxyphosphinylthiomethyl)] 4-pyrone **E24**
 4-methoxy-3,3'-dimethylbenzophenone **M145**
 methoxydiuron **L50**

3-methoxy-1,2-epoxypropane **G32**
 methoxyethane **E147**
 2-methoxyethanol **M134**
 2-methoxyethanol acetate **M136**
 methoxyethene **M317**
 2-(2-methoxyethoxy)ethanol **M135**
 2-[2-(2-methoxyethoxy)ethoxy]ethanol **T283**
 2-methoxyethyl acetate **M136**
 2-methoxy-4-ethylamino-6-*tert*-butylamino-s-triazine **T23**
 S-[2-[(2-methoxyethyl)amino]-2-oxoethyl] *O,O*-dimethyl phosphorodithioic acid ester **A110**
 S-(*N*-2-methoxyethylcarbamoylmethyl)-*O,O*-dimethyl dithiophosphate **A110**
 methoxyethylene **M317**
 (2-methoxyethyl) ether **D338**
 2-methoxyethylmercury acetate **M137**
 methoxyethylmercury(II) acetate **M137**
 methoxyfluorane **M138**
 9-methoxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one **M129**
 6-methoxyguanine **M139**
 6-methoxyharman **H7**
 methoxyhexanone **M140**
 2-methoxy-1-hydroxy-4-allylbenzene **E187**
 3-methoxy-4-hydroxybenzaldehyde **V17**
N-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]acetamide **M48**
 1-(2-methoxyisopropoxy)-2-propanol **D556**
 methoxylene **M118**
 methoxymethane **D413**
 2-methoxy-5-methylaniline **C455**
 4-methoxy-2-methylaniline **C454**
 2-methoxy-5-methylbenzenamine **C455**
 4-methoxy-2-methylbenzenamine **C454**
 methoxymethylbenzene **M166**
 1-methoxy-4-methylbenzene **M157**
N-(methoxymethyl)-2,6-diethyl-2-chloroacetanilide **A60**
 (2-methoxymethylthoxy)propanol **D556**
 3-methoxy-17-methylmorphinan, (9 α ,13 α ,14 α)- **D63**
 α -(methoxymethyl)-2-nitroimidazole-1-ethanol **M335**
 α -(methoxymethyl)-2-nitro-1*H*-imidazole-1-ethanol **M335**
 (methoxymethyl)oxirane **G32**
 3-methoxy-5-methyl-4-oxo-2,5-hexadienoic acid, **P21**
 3-(3-methoxy-2-methyl-3-oxo-1-propenyl)-2,2-dimethyl-cyclopropanecarboxylic acid 2-methyl-4-oxo-3-(2-pentenyl)-2-cyclopenten-1-yl ester, [1*R*-[1 α [*S**(*Z*)],3 β (*E*)]- **J2**
 4-methoxy-4-methyl-2-pentanone **M140**
 4-methoxy-4-methylpentan-2-one **M140**
 (4-methoxy-3-methylphenyl)(3-methylphenyl)-methanone **M145**
 2-methoxy-2-methylpropane **M181**
 7-methoxy-1-methyl-9*H*-pyrido[3,4-*b*]indole **H7**
 (+)-2-(6-methoxy-2-naphthyl)propionic acid **N29**
d-2-(6-methoxy-2-naphthyl)propionic acid **N29**
 2-methoxy-4-nitroaniline **M141**
 2-methoxy-5-nitroaniline **M142**
 4-methoxy-2-nitroaniline **M143**
 2-methoxy-4-nitrobenzenamine **M141**
 2-methoxy-5-nitrobenzenamine **M142**
 4-methoxy-2-nitrobenzenamine **M143**
 1-methoxy-2-nitrobenzene **N77**
 1-methoxy-3-nitrobenzene **N78**
 1-methoxy-4-nitrobenzene **N79**
 2-methoxynitrobenzene **N77**
 3-methoxynitrobenzene **N78**
 4-methoxynitrobenzene **N79**
 2-methoxy-*N*-(2-oxo-1,3-oxazolidin-3-yl)acet-2',6'-xylidide **O45**
 S-[(5-methoxy-2-oxo-1,3,4-thiadiazol-3(2*H*)-yl)methyl] *O,O*-dimethyl phosphorodithioate **M121**
 4-methoxyphenol **M144**
p-methoxyphenol **M144**
 methoxyphenone **M145**
 3-(2-methoxyphenoxy)-1-glyceryl carbamate **M125**
 3-[*p*-(*p*-methoxyphenoxy)phenyl]-1,1-dimethylurea **D324**
N'-[4-(4-methoxyphenoxy)phenyl]-*N,N*-dimethylurea **D324**
 3-(2-methoxyphenoxy)-1,2-propanediol **G47**
 3-(*o*-methoxyphenoxy)-1,2-propanediol 1-carbamate **M125**
p-methoxyphenylamine **A215**
 methoxyphenylenediamine **D73**
 4-methoxy-1,3-phenylenediamine **D73**
 4-methoxy-*m*-phenylenediamine **D73**
 4-methoxy-*m*-phenylenediamine sulfate **D74**
 1-methoxypropane **M291**
 methoxypropanol **M146**
 1-methoxypropan-2-ol **M147**
 1-methoxy-2-propanol **M147**
 (\pm)-1-methoxypropan-2-ol **M147**
 1-methoxy-2-propanol acetate **M148**
 1-methoxypropan-2-ol acetate **M148**
 2-methoxypropanol acetate **M149**
 1-methoxy-2-propanone **M131**
 1-methoxy-4-(2-propenyl)benzene **A75**
 2-methoxy-4-(1-propenyl)phenol **I102**
 2-methoxypropyl acetate **M149**
 3-methoxypropyl oxide **G32**
 8-methoxypsoralen **M129**
 6-methoxy-1*H*-purin-2-amine **M139**
 α -methoxytoluene **M166**
p-methoxytoluene **M157**
 methoxytriethylene glycol **T283**
 (3 β ,16 β ,17 α ,18 β ,20 α)-17-methoxy-18-[(3,4,5-trimethoxybenzoyl)oxy]-yohimban-16-carboxylic acid, methyl ester **D58**
 Methrazone **F29**
 methulose **M185**
N,N'-methylenyl-*o*-phenylenediamine **B53**
 methylacetaldehyde **P309**
 methylacetamide **M150**
N-methylacetamide **M150**
 methyl acetate **M151**
 methylacetic acid **P310**

methylacetic anhydride **P311**
 methyl acetoacetate **M152**
 3-methylacetoacetone **M276**
 methylacetone **M220**
 (Z)-2'-methylacetophenone 4,6-dimethylpyrimidin-2-ylhydrazone **F31**
 methylacetopyranone **D45**
 methyl acetylacetate **M152**
 methylacetylene **P338**
 methyl acid **T173**
 2-methylacrolein **M103**
 β-methylacrolein **C467**
 2-methylacrylamide **M105**
 methyl acrylate **M153**
 3-methylacrylic acid **C468**
 methyladronal **M201**
 methylal **D382**
 methyl alcohol **M116**
 methylaldehyde **F100**
 1-methylallyl alcohol **B220**
 2-methylallyl alcohol **M289**
 3-methylallyl alcohol **C470**
 γ-methylallyl chloride **C176**
 methylamine **M154**
 (methylamino)benzene **M156**
 methyl 4-aminobenzene sulfonylcarbamate **A251**
 O-[(methylamino)carbonyl]oxime **A62**
 N-[[[(methylamino)carbonyl]oxy]ethanimidothioic acid, methyl ester **M126**
 N-methylaminodithioformic acid, sodium salt **M96**
 2-(methylamino)ethanol **M155**
 N-methyl-2-aminoethanol **M155**
 methylaminoethanolcatechol **A51**
 (1R,2S)-(α-(1-methylamino)ethyl)benzyl alcohol **E30**
 1-[α-(1-methylamino)ethyl]benzyl alcohol sulfate **E31**
 (Z)-3-(methylamino)-1-methyl-1-oxo-1-propenyl dimethyl phosphate **D429**
 p-(methylamino)nitrobenzene **M263**
 6-methyl-2-(p-aminophenyl)-7-benzothiazole sulfonic acid **A146**
 methyl 4-aminophenylsulfonylcarbamate **A251**
 methyl ((4-aminophenyl)sulfonyl)carbamate **A251**
 methylaminopterin **M128**
 methylamyl acetate **H77**
 methylamyl alcohol **M277**
 methyl amyl ketone **H23**
 methyl n-amyl ketone **H23**
 2-methylaniline **T185**
 3-methylaniline **T184**
 4-methylaniline **T187**
 N-methylaniline **M156**
 o-methylaniline hydrochloride **T186**
 2-methyl-p-anisidine **C454**
 5-methyl-o-anisidine **C455**
 4-methylanisole **M157**
 p-methylanisole **M157**
 methylanol **M201**

methylanone **M203**
 2-methyl-1-anthraquinonylamine **A130**
 methylapoxide **M99**
 2-methylaziridine **M158**
 4-[(methylazo)methyl]-N-(1-methylethyl)-benzamide **A272**
 methylazoxymethanol **M159**
 (methyl-O,N,N-azoxy)methanol **M159**
 methylazoxymethanol acetate **M160**
 (methyl-O,N,N-azoxy)methanol, acetate (ester) **M160**
 methylazoxymethanol β-D-glucoside **C494**
 methylazoxymethyl acetate **M160**
 (methyl-O,N,N-azoxy)methyl β-D-glucopyranoside **C494**
 2-methylbenzenamine **T185**
 3-methylbenzenamine **T184**
 4-methylbenzenamine **T187**
 N-methylbenzenamine **M156**
 2-methylbenzenamine, hydrochloride **T186**
 methylbenzene **T173**
 methyl benzeneacetate **M286**
 2-methylbenzenecarbonitrile **T189**
 2-methyl-1,3-benzenediamine **D90**
 2-methyl-1,4-benzenediamine **D88**
 3-methyl-1,2-benzenediamine **D86**
 4-methyl-1,2-benzenediamine **D92**
 4-methyl-1,3-benzenediamine **D87**
 5-methyl-1,3-benzenediamine **D93**
 2-methyl-1,4-benzenediamine sulfate **D89**
 2-methyl-1,4-benzenediamine, sulfate **T174**
 (±)-α-methylbenzene ethanamine **A193**
 α-methylbenzenemethanol **P68**
 4-methylbenzenesulfonic acid **T179**
 4-methylbenzenesulfonic acid, methyl ester **M313**
 4-methylbenzenesulfonyl chloride **T180**
 methyl benzoate **M161**
 2-methylbenzoic acid **T182**
 3-methylbenzoic acid **T181**
 4-methylbenzoic acid **T183**
 m-methylbenzoic acid **T181**
 methylbenzol **T173**
 2-methylbenzonitrile **T189**
 3-methylbenzonitrile **T188**
 4-methylbenzonitrile **T190**
 2-methylbenzothiazole **M162**
 p-(6-methylbenzothiazol-2-yl)aniline **A145**
 4-(6-methyl-2-benzothiazolyl)benzenamine **A145**
 methylbenzotriazole **M164**
 methyl-1H-benzotriazole **M164**
 1-methylbenzotriazole **M163**
 1-methyl-1H-benzotriazole **M163**
 4(or 5)-methylbenzotriazole **M164**
 4(or 5)-methyl-1H-benzotriazole **M164**
 5-methylbenzotriazole **M165**
 5-methyl-1,2,3-benzotriazole **M165**
 5-methyl-1H-benzotriazole **M165**
 methyl N-benzoyl-N-(3-chloro-4-fluorophenyl)alaninate **F34**

α -methylbenzyl alcohol **P68**
 methyl benzyl ether **M166**
 α -methylbenzyl 3-hydroxycrotonate, dimethyl phosphate **M167**
 3-methyl-9-benzyl-1,2,3,4-tetrahydro- γ -carboline **M36**
N-methyl-9-benzyl tetrahydro- γ -carboline **M36**
 methylbiphenyl **M168**
 methyl-1,1'-biphenyl **M168**
 2-methylbiphenyl **M169**
 2-methyl-1,1'-biphenyl **M169**
 4-methylbiphenyl **M170**
 4-methyl-1,1'-biphenyl **M170**
 [1 α ,3 α Z]-(\pm)-(2-methyl[1,1'-biphenyl]-3-yl)methyl 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethylcyclopropanecarboxylate **B109**
 2-methylbiphenyl-3-ylmethyl Z-(1*RS*,3*RS*)-3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethylcyclopropane-carboxylate **B109**
 methylbis(2-chloroethyl)amine **M38**
 methylbis(β -chloroethyl)amine *N*-oxide **M39**
 2-methyl-1,2-bis(3-pyridyl)-1-propanone **M329**
 2-methylbiviny **I115**
 methyl borate **T308**
 methyl bromide **B178**
 methyl bromoacetate **M171**
 1-methylbutadiene **P34**
 2-methylbutadiene **I115**
 2-methyl-1,3-butadiene **I115**
N-methylbutamine **M180**
 2-methylbutanal **M183**
 3-methylbutanal **I140**
 α -methylbutanal **M183**
 2-methylbutane **M172**
 2-methylbutane-*sec*-mononitrile **I142**
 3-methylbutanenitrile **I142**
 3-methylbutanoic acid **I141**
 3-methylbutanoic acid, allyl ester **A88**
 3-methylbutanoic acid, butyl ester **B265**
 3-methylbutanoic acid, methyl ester **M246**
 3-methylbutanoic acid, 2-propenyl ester **A88**
 2-methylbutan-2-ol **M173**
 2-methyl-2-butanol **M173**
 3-methylbutan-1-ol **M174**
 3-methyl-1-butanol **M174**
 2-methyl-2-butanol acetate **A196**
 methylbutanone **M244**
 3-methylbutan-2-one **M244**
 2-methyl-2-butene **A200**
 3-methylbut-1-ene **M175**
 3-methyl-1-butene **M175**
 (*E*)-2-methyl-2-butenic acid **T157**
 2-methyl-2-butenic acid 7-[(2,3-dihydroxy-2-(1-methoxyethyl)-3-methyl-1-oxobutoxy)methyl]-2,3,5,7a-tetrahydro-1*H*-pyrrolizin-1-yl ester, [1*S*-[1 α (*Z*),7(2*S**,3*R**),7 α]]- **L6**
 2-methyl-3-buten-2-ol **M178**
 3-methyl-2-buten-1-ol **M176**
 3-methylbut-2-en-1-ol **M176**
 3-methyl-3-buten-1-ol **M177**
 3-methyl-3-buten-2-one **M179**
 4-(3-methyl-2-butenyl)-1,2-diphenyl-3,5-pyrazolidinedione **F29**
 1-methylbutyl acetate **P46**
 3-methylbutyl acetate **I80**
 methylbutylamine **M180**
N-methylbutylamine **M180**
 methyl 1-[(butylamino)carbonyl]-1*H*-benzimidazol-2-ylcarbamate **B32**
 1-methyl-4-*tert*-butylbenzene **B278**
p-methyl-*tert*-butylbenzene **B278**
 3-methylbutyl bromide **B179**
 methyl 1-(butylcarbomoyl)-2-benzimidazolecarbamate **B32**
 methyl 1-(butylcarbomoyl)benzimidazol-2-ylcarbamate **B32**
 2-(1-methylbutyl)-4,6-dinitrophenol **D509**
 methyl *tert*-butyl ether **M181**
 methyl butyl ketone **H67**
 methyl *n*-butyl ketone **H67**
 2-methyl-3-(4-*tert*-butylphenyl)propionaldehyde **L44**
 5-(1-methylbutyl)-5-(2-propenyl)-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione **Q3**
 2-methyl-3-butyne-2-ol **M182**
 methylbutyraldehyde **M183**
 2-methylbutyraldehyde **M183**
 3-methylbutyraldehyde **I140**
 2-methylbutyric aldehyde **M183**
 4-methylbutyrolactone **V3**
 3-methylbutyronitrile **I142**
 methylcaptopax **M309**
 methyl carbamate **M184**
 methylcarbamate, 1-naphthyl- **C63**
 methyl carbamate with eseroline **P178**
 methylcarbamic acid, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl ester **C68**
 methylcarbamic acid, 2,3-dihydro-2-methyl-7-benzofuranyl ester **D43**
 methylcarbamic acid, 4-dimethylamino-*m*-tolyl ester **A123**
 methylcarbamic acid, *o*-isopropoxyphenyl ester **P315**
 methylcarbamic acid, 2,3-(isopropylidenedioxy)phenyl ester **B28**
 methylcarbamic acid, 4-(methylthio)-3,5-xylyl ester **M123**
 methylcarbamic acid, 2,3,4-trimethylphenyl ester **T300**
 methylcarbomodithioic acid, sodium salt **M96**
O-(methylcarbomoyl)oxime **A62**
N-[(methylcarbomoyl)oxy]thioacetimidic acid, methyl ester **M126**
 3-(methylcarbomoyl)pyridine **M297**
 methyl carbitol **M135**
 2-methyl- β -carboline **H6**
 3-methyl-4-carboline **H6**
 methyl carbomethoxybenzoate **D459**
 methylcarbonitrile **A20**

methyl carbonochloridate **M188**
 methyl cellosolve **M134**
 methyl cellosolve acetate **M136**
 methylcellulose **M185**
 O-methyl cellulose **M185**
 methyl cellulose ether **M185**
 methylchavicol **A75**
 Methyl Chemosept **M272**
 methyl chloride **C206**
 methyl chloroacetate **M186**
 methyl 2-chloroacrylate **M187**
 2-methylchlorobenzene **C288**
 3-methylchlorobenzene **C289**
 4-methylchlorobenzene **C290**
 O-methyl-O-2-chloro-4-*tert*-butylphenyl-N-methylamido-phosphate **C471**
 methyl chlorocarbonate **M188**
 4-methyl-5-(β -chloroethyl)thiazole **C360**
 methylchloroform **T247**
 methyl chloroformate **M188**
 methyl chlorofos **T225**
 methyl 2-chloro-9-hydroxyfluorene-9-carboxylate **C129**
 methyl chloromethyl ether **C214**
 2-methyl-4-chlorophenoxyacetic acid **M32**
 N'-(2-methyl-4-chlorophenyl)-N,N-dimethylformamidine **C121**
 methylchloropindol **C363**
 methyl 2-chloro-2-propenoate **M187**
 methyl 2-chloropropionate **M189**
 methyl α -chloropropionate **M189**
 methylchlorotetracycline **D47**
 (2*S*-*trans*)-methyl-7-chloro-6,7,8-trideoxy-6-[(1-methyl-4-propyl-2-pyrrolidinyl)carbonyl]amino]-1-thio-L-threo- α -D-galacto-octopyranoside **C354**
 20-methylcholanthrene **M190**
 3-methylcholanthrene **M190**
 1-methylchrysene **M191**
 2-methylchrysene **M192**
 3-methylchrysene **M193**
 5-methylchrysene **M194**
 6-methylchrysene **M195**
 6-methyl-*m*-cresol **X11**
 (E)-2-methylcrotonic acid **T157**
 (E)- α -methylcrotonic acid **T157**
trans-2-methylcrotonic acid **T157**
 5-methyl-*m*-cumenyl methylcarbamate **P286**
 methyl cyanide **A20**
 methyl 2-cyanoacrylate **M196**
 4-methylcyanobenzene **T190**
 methyl 2-cyano-2-propenoate **M196**
 methylcyclohexane **M197**
 methylcyclohexanol **M198**
 2-methylcyclohexanol **M199**
 3-methylcyclohexanol **M200**
 3-methyl-1-cyclohexanol **M200**
 4-methylcyclohexanol **M201**
 4-methyl-1-cyclohexanol **M201**
m-methylcyclohexanol **M200**
p-methylcyclohexanol **M201**
 methylcyclohexanone **M202**
 methylcyclohexan-1-one **M202**
 1-methylcyclohexan-2-one **M203**
 2-methylcyclohexanone **M203**
 2-methylcyclohexyl alcohol **M199**
 4-methylcyclohexyl alcohol **M201**
 1-(2-methylcyclohexyl)-3-phenylurea **S27**
 N-(2-methylcyclohexyl)-N'-phenylurea **S27**
 2-methylcyclopentadienyl manganesetricarbonyl **M25**
 methylcyclopentane **M204**
 methylcymantrene **M25**
 methyl 11-demethoxy-18-O-(3,4,5-trimethoxybenzoyl)-reserpate **D58**
 methyl demeton **D50**
 methyl dichloroacetate **M205**
 methyl α ,4-dichlorobenzenepropanoate **C126**
 methyl *p*, α -dichlorohydrocinnamate **C126**
 methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate **B108**
 methyl 2-[4-(2,4-dichlorophenoxy)phenoxy]propanoate **D259**
 methyl dichlorosilane **D225**
 methyl diethanolamine **M206**
 methyl diethyl carbinol **M279**
 4-methyl-2,3-dihydrofuran **D345**
 α -methyl dihydroindole **M239**
 methyl (E)-3-(dimethoxyphosphinothioyl)-2-methylacrylate **M102**
 (E)-methyl 3-[(dimethoxyphosphinothioyl)oxy]-2-methylpropenoate **M102**
 methyl 3-(dimethoxyphosphinyloxy)crotonate **M330**
 methyl 1,1-dimethylethyl ether **M181**
 methyl N-(2,6-dimethylphenyl)-N-(2-furanylcarbonyl)-DL-alaninate **F119**
 methyl N-(2,6-dimethylphenyl)-N-(2-furoyl)-DL-alaninate **F119**
 methyl-N-(2,6-dimethylphenyl)-N-(phenylacetyl)-DL-alaninate **B26**
 methyl 2,2-dimethylvinyl ketone **M91**
 methyl dimuron **M209**
 2-methyl-3,5-dinitrobenzamide **D465**
 methyl dinitrobenzene **D497**
 1-methyl-2,3-dinitrobenzene **D498**
 1-methyl-2,4-dinitrobenzene **D499**
 1-methyl-2,6-dinitrobenzene **D501**
 1-methyl-3,5-dinitrobenzene **D503**
 2-methyl-1,3-dinitrobenzene **D501**
 2-methyl-1,4-dinitrobenzene **D500**
 4-methyl-1,2-dinitrobenzene **D502**
 2-methyl-4,6-dinitrophenol **D475**
 4-methyl-2,6-dinitrophenol **D474**
 N-methyl-N,4-dinitrosoaniline **M207**
 N-methyl-N,4-dinitrosobenzenamine **M207**
 N-methyl-2,4-dinitro-N-(2,4,6-tribromophenyl)-6-(trifluoromethyl)benzenamine **B153**
 2-methyldiphenhydramine **O35**

o-methyldiphenhydramine **O35**
 4-methyldiphenyl **M170**
 2-methyl-1,2-di-3-pyridinyl-1-propanone **M329**
 6-methyl dipyrrodo[1,2-*a*:3',2'-*d*]imidazol-2-amine **G19**
 2-methyl-1,2-di-3-pyridyl-1-propanone **M329**
 methyl disulfide **D412**
 methylthiocarbamic acid, sodium salt **M96**
 (4-methyl-1,3-dithiolan-2-ylidene)phosphoramidic acid, diethyl ester **M56**
 6-methyl-1,3-dithiolo[4,5-*b*]quinoxalin-2-one **Q11**
 methylthiomethane **D412**
 2-methyl-1,3-di(2,4-xylylimino)-2-azapropane **A158**
 methyl dopa **M208**
 methyl dymron **M209**
 methylene acetone **M318**
 2,2'-methylenebiphenyl **F49**
 methylenebis(4-aminocyclohexane) **D272**
 2,4'-methylenebis(aniline) **M217**
 4,4'-methylenebisbenzenamine **M218**
 1,1'-methylenebis(benzene) **D547**
 methylenebis(3-chloro-4-aminobenzene) **M210**
 4,4'-methylenebis(2-chloroaniline) **M210**
 4,4'-methylenebis(*o*-chloroaniline) **M210**
 4,4'-methylenebis(2-chlorobenzenamine) **M210**
 2,2'-methylenebis(4-chlorophenol) **D235**
 4,4'-methylenebiscyclohexanamine **D272**
 4,4'-methylenebiscyclohexylamine **D272**
 4,4'-methylenebis(cyclohexyl isocyanate) **M211**
 methylenebis(4-cyclohexyl isocyanate) **M211**
 methylene-*S,S'*-bis(*O,O*-diethyldithiophosphate) **E68**
 4,4'-methylenebis(*N,N*-dimethylaniline) **M212**
 4,4'-methylenebis(*N,N*-dimethylbenzenamine) **M212**
 3,3'-methylenebis(4-hydroxy-2*H*-1-benzopyran-2-one) **D262**
 3,3'-methylenebis(4-hydroxycoumarin) **D262**
 1,1'-methylenebis(4-isocyanatobenzene) **M214**
 1,1'-methylenebis(4-isocyanatocyclohexane) **M211**
 4,4'-methylenebis(2-methylaniline) **M213**
 4,4'-methylenebis(2-methylbenzenamine) **M213**
 1,1'-methylenebis(oxy)bis(2-chloroethane) **B118**
 1,1'-[methylenebis(oxy)]bisethane **D286**
 4,4'-methylenebis(phenyl isocyanate) **M214**
 methylenebis[4-phenyl isocyanate] **M214**
 1,1'-methylenebis(thiosemicarbazide) **M215**
 4,4'-methylenebis(*o*-toluidine) **M213**
 2,2'-methylenebis(3,4,6-trichlorophenol) **H41**
 Methylene Blue **M216**
 methylene bromide **D133**
 methylenebutanedioic acid **I144**
 methylene chloride **D222**
 methylene chlorobromide **B171**
 methylene cyanide **M18**
 2,4'-methylenedianiline **M217**
 4,4'-methylenedianiline **M218**
 4,4'-methylenedianiline dihydrochloride **M219**
 4,4'-methylenedibenzenamine dihydrochloride **M219**
 methylene dibromide **D133**
 methylene dichloride **D222**
 methylenediethanolamine **M206**
 methylenedinitrile **M18**
 1,5-methylene-3,7-dinitroso-1,3,5,7-tetraazacyclooctane **D495**
 1,2-methylenedioxy-4-[2-(octylsulfinyl)propyl]benzene **S148**
 1,2-(methylenedioxy)-4-propenylbenzene **I136**
 1,2-(methylenedioxy)-4-propylbenzene **D347**
 3,4-methylenedioxypropylbenzene **D347**
 (3,4-methylenedioxy-6-propylbenzyl)(butyl) diethylene glycol ether **P204**
 4,4'-methylenediphenyl diisocyanate **M214**
 4-methylene-2-oxetanone **D363**
 methylene oxide **F100**
 4,5-methylenephenanthrene **C526**
 methylenesuccinic acid **I144**
 methylenium ceruleum **M216**
 methyl ethanoate **M151**
N-methylethanolamine **M155**
 methylethene **P303**
 (1-methylethenyl)benzene **M307**
 2-methyl-5-ethenylpyridine **M319**
 methyl ether **D413**
 methyl ether of propylene glycol **M146**
 methyl ethoxol **M134**
 2-(1-methylethoxy)ethanol **I119**
 methyl 2-[[[4-ethoxy-6-(methylamino)-1,3,5-triazin-2-yl]amino]carbonyl]amino]sulfonyl]benzoate **E57**
 methyl 2-[(4-ethoxy-6-methylamino-1,3,5-triazin-2-yl)carbamoysulfamoyl]benzoate **E57**
 2-(1-methylethoxy)phenol methylcarbamate **P315**
 2-(1-methylethoxy)phenyl methylnitrosocarbamate **N173**
N-[3-(1-methylethoxy)phenyl]-2-(trifluoromethyl)benzamide **F92**
 1-methylethyl acetate **I120**
 1-methylethylamine **I121**
 1-[(1-methylethyl)amino]-3-(1-naphthalenyloxy)-2-propanol **P321**
 1-[(1-methylethyl)amino]-3-[2-(2-propenyloxy)phenoxy]-2-propanol **O52**
 4-(1-methylethyl)benzaldehyde **I122**
 (1-methylethyl)benzene **C474**
 1-methyl-2-ethylbenzene **E176**
 1-methyl-3-ethylbenzene **E177**
 1-methyl-4-ethylbenzene **E178**
 3-(1-methylethyl)-(1*H*)-2,1,3-benzothiadiazin-4(3*H*)-one-2,2-dioxide **B38**
 (*R*)-1-methylethyl *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)-alaninate **F35**
 methylethylbromomethane **B165**
 methyl ethyl carbinol **B213**
 1-methylethylcyclohexane **I125**
 4-(1-methylethyl)-2,6-dinitro-*N,N*-dipropylbenzenamine **I117**
 methylethylene **P303**

methylethylene oxide **P330**
 2-methylethylenimine **M158**
 1-methylethyl ethanoate **I120**
 methylethyl glycol **P327**
 (R)-2-[[[(1-methylethylidene)amino]oxy]ethyl 2-[4-[(6-chloro-2-quinoxalinyloxy]phenoxy]propanoate **P299**
 4,4'-(1-methylethylidene)bis(2,6-dibromophenol) **T39**
 4,4'-(1-methylethylidene)bisphenol **B133**
 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxy-methylene)]bisoxirane **B134**
 2-(1-methylethylidene)hydrazine carbothioamide **A19**
 methyl ethyl ketone **M220**
 methyl ethyl ketone hydroperoxide **M222**
 methyl ethyl ketone oxime **M221**
 methyl ethyl ketone peroxide **M222**
 methyl ethyl ketoxime **M221**
 (E,E)-1-methylethyl 11-methoxy-3,7,11-trimethyl-2,4-dodecadienoate **M127**
 N-(1-methylethyl)-4-[(2-methylhydrazino)methyl]-benzamide **I1**
 1-methylethyl 2-(1-methylpropyl)-4,6-dinitrophenyl carbonate **D504**
 2-(1-methylethyl)naphthalene **I128**
 1-(1-methylethyl)-4-nitrobenzene **N109**
 methylethyl nitrosamine **N161**
 N,N-methylethyl nitrosamine **N161**
 N-(1-methylethyl)-N-nitroso-2-propanamine **N152**
 2-(1-methylethyl)-4-pentenamide **A86**
 4-(1-methylethyl)phenol **I130**
 3-(1-methylethyl)phenol methyl carbamate **I131**
 2-(1-methylethyl)phenyl methyl carbamate **I116**
 (1-methylethyl)phosphoramidic acid ethyl 3-methyl-4-(methylthio)phenyl ester **F3**
 N-(1-methylethyl)-2-propanamine **D358**
 5-methyl-2-ethylpyrazine **E149**
 2-methyl-5-ethylpyridine **E163**
 1-(1-methylethyl)-1H-pyrrole-2,5-dione **I127**
 α -(1-methylethyl)- α -[4-(trifluoromethoxy)phenyl]-5-pyrimidine methanol **F89**
 methyleugenol **M223**
 methyl fluorosulfate **M224**
 methyl fluorosulfonate **M224**
 Methylflurether **E27**
 N-methylformamide **M225**
 methyl formate **M226**
 N-methyl-N-formylhydrazine **M227**
 2-methylfuran **M228**
 5-methylfuran **M228**
 α -methylfuran **M228**
 2-methyl-3-furanilide **F10**
 methyl N-(2-furoyl)-N-(2,6-xylyl)-DL-alaninate **F119**
 methyl glycidyl ether **G32**
 methyl glycol acetate **M136**
 methylglycolic acid **M130**
 methyl glycol monoacetate **M136**
 O⁶-methylguanine **M139**
 1-methyl-1-heptanol **O14**
 6-methyl-1-heptanol **M229**
 5-methylheptan-3-one **M230**
 5-methyl-3-heptanone **M230**
 methylheptenone **M231**
 2-methyl-2-hepten-6-one **M232**
 6-methyl-5-hepten-2-one **M232**
 6-methyl- Δ^5 -hepten-2-one **M232**
 methylhexabital **H76**
 methylhexalin **M198**
 5-methylhexan-2-one **M233**
 5-methyl-2-hexanone **M233**
 methylhexylcarbinol **O14**
 methyl hexyl ketone **O16**
 methylhydrazine **M234**
 methylhydrazine monosulfate **M235**
 methylhydrazine sulfate **M235**
 4-[(2-methylhydrazino)methyl]-N-isopropylbenzamide **P274**
 methyl hydride **M112**
 methyl hydroxide **M116**
 methyl 2-hydroxybenzoate **M305**
 methyl *p*-hydroxybenzoate **M272**
 2-methyl-3-hydroxy-4,5-bis(hydroxymethyl)pyridine hydrochloride **P359**
 N-methyl-2-hydroxyethylamine **M155**
 2-methyl-2-*p*-hydroxyphenylbutane **A205**
 methyl 2-hydroxypropanoate **M247**
 methyl 17-hydroxy-yohimban-16-carboxylate **Y1**
 1,1',1'-(methylidyne)tris(oxy)tris(ethane) **T286**
 1-methylimidazole **M236**
 1-methyl-1*H*-imidazole **M236**
 1-methylimidazole-2-thiol **M122**
 2,2'-(methylimino)bisethanol **M206**
 methyliminodiethanol **M206**
 2,2'-(methylimino)diethanol **M206**
 N,N'-[(methylimino)dimethylidyne]di-2,4-xylylidine **A158**
 β -methylmipramine **T328**
 5-methylindan **M237**
 3-methylindole **M238**
 β -methylindole **M238**
 2-methylindoline **M239**
 methyl iodide **I52**
 methylisoamyl acetate **H77**
 methyl isoamyl ketone **M233**
 2-methylisoborneol **M240**
 methyl isobutenyl ketone **M91**
 methyl isobutyl carbinol **M277**
 methylisobutylcarbinol acetate **H77**
 methyl isobutyl ketone **M241**
 methylisobutylxanthine **I93**
 methyl isobutyrate **M242**
 methyl isocyanate **M243**
 methyl isopentanoate **M246**
 methyl isopentyl ketone **M233**
 methyl isopropenyl ketone **M179**
 1-methyl-4-isopropylbenzene **C540**

1-methyl-4-isopropyl-1,3-cyclohexadiene **T34**
 5-methyl-2-isopropylcyclohexanol **M53**
 1-methyl-4-isopropylidene-1-cyclohexene **T37**
 methyl isopropyl ketone **M244**
 methyl isothiocyanate **M245**
 methyl isovalerate **M246**
 3-methyl-4,5-isoxazolidione, 4-(2-chlorophenyl)hydrazone **D600**
 3-methyl-4,5-isoxazolidione 4-[(*o*-chlorophenyl)hydrazone] **D600**
 5-methylisoxazol-3-ol **H121**
 5-methyl-3-isoxazolol **H121**
 5-methyl-3(2*H*)-isoxazalone **H121**
N'-(5-methyl-3-isoxazolyl)sulfanilamide **S136**
 methyl lactate **M247**
 methyl lactonitrile **A18**
 2-methylactonitrile **A18**
 methyl maleate **D426**
 methyl mercaptan **M115**
 methyl mercaptoacetate **M248**
 2-(methylmercapto)benzothiazole **M309**
 methyl-mercaptosulfonate **D52**
 methylmercaptosulfonate **D52**
 methyl mercaptoimidazole **M122**
 methylmercuric acetate **M250**
 methylmercuric cyanoguanidine **M251**
 methylmercury **M249**
 methylmercury(1+) **M249**
 methylmercury(II) acetate **M250**
 methylmercury(II) dicyanamide **M251**
 methylmercury(II) dicyandiamide **M251**
 methylmercury ion(1+) **M249**
 methyl mesylate **M253**
 methyl methacrylate **M252**
 methyl methacrylate homopolymer **P226**
N-methylmethanamine **D384**
 methylmethane **E58**
 methyl methanesulfonate **M253**
 methyl methanesulfonic acid **M253**
 methyl methanoate **M226**
 2-methyl-2-(methylsulfonyl)propanal *O*-(methylcarbamoyl)-oxime **A64**
 methyl *N*-(methoxyacetyl)-*N*-(2,6-xylyl)-DL-alaninate **M93**
 methyl (*N*-(2-methoxyacetyl)-*N*-(2,6-xylyl)-DL-alaninate **M93**
 2-methyl-4-methoxyaniline **C454**
 1-methyl-7-methoxy- β -carboline **H7**
 3-[2-methyl-3-(methoxy carbonyl)-1-propenyl]-2,2-dimethylcyclopropanecarboxylic acid, 3-(2-butenyl)-2-methyl-4-oxo-2-cyclopenten-1-yl ester **C345**
 methyl *p*-methylbenzenesulfonate **M313**
 5-methyl *N*-[methylcarbamoyl]oxythioacetimidate **M126**
 1-methyl-1-(4-methylcyclohexyl)ethyl hydroperoxide **M52**
 1-methyl-2-(3,4-methylenedioxyphenyl)ethyloctyl sulfoxide **S148**
 methylmethylene glycol **B203**
 7-methyl-3-methylene-1,6-octadiene **M361**
 5-methyl-2-(1-methylethenyl)cyclohexanol, [1*R*-(1 α ,2 β ,5 α)]- **I134**
 1-methyl-4-(1-methylethenyl)cyclohexene **L45**
 1-methyl-4-(1-methylethenyl)cyclohexene, (*R*)- **L46**
 2-methyl-*N*-[3-(1-methylethoxy)phenyl]benzamide **M58**
 methyl(1-methylethyl)benzene **C537**
 1-methyl-4-(1-methylethyl)-1,3-cyclohexadiene **T34**
 1-methyl-4-(1-methylethyl)-*trans*-cyclohexane **M51**
 5-methyl-2-(1-methylethyl)cyclohexanol **M53**
 5-methyl-2-(1-methylethyl)cyclohexanol, (1 α ,2 β ,5 α)-(±)- **M54**
 1-methyl-4-(1-methylethylidene)cyclohexane **T37**
N-methyl-*N*1-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine **D60**
 2-methyl-4-(1-methylethyl)-7-oxo-8-oxa-3-thia-2,4-diazadecanoic acid 2,3-dihydro-2,2-dimethyl-7-benzofuranyl ester **B30**
 5-methyl-2-(1-methylethyl)phenol **T154**
 3-methyl-5-(1-methylethyl)phenol methylcarbamate **P286**
 2-methyl-3-(2-methylphenyl)-4-quinazolinone **M119**
 2-methyl-3-(2-methylphenyl)-4(3*H*)-quinazolinone **M119**
 methyl 2-methylpropenoate **M252**
 methyl 2-methyl-2-propenoate, homopolymer **P226**
 2-methyl-2-methylpropionaldehyde *O*-methylcarbamoyloxime **A64**
 α -methyl-4-(2-methylpropyl)benzeneacetic acid **I2**
 2-methyl-*N*-(2-methylpropyl)-1-propanamine **D352**
 2-methyl-2-methyl sulfonyl propionaldehyde *O*-methylcarbamoyloxime **A64**
 2-methyl-2-methylsulfonylpropionaldehyde *O*-methylcarbamoyloxime **A64**
 3-methyl-4-(methylthio)phenol **M254**
 2-methyl-2-(methylthio)propanol **A62**
 2-methyl-2-(methylthio)propionaldehyde **A62**
 methyl monochloroacetate **M186**
 4-methylmorpholine **M255**
N-methylmorpholine **M255**
 methyl mustard oil **M245**
 methylnaftalen **M256**
 methyl namate **S64**
 methylnaphthalene **M256**
 1-methylnaphthalene **M257**
 2-methylnaphthalene **M258**
 α -methylnaphthalene **M257**
 β -methylnaphthalene **M258**
N-methylnicotinamide **M297**
 2-methyl-4-nitroaniline **M259**
 2-methyl-5-nitroaniline **M260**
 4-methyl-2-nitroaniline **M261**
 4-methyl-3-nitroaniline **M262**
N-methyl-4-nitroaniline **M263**
 2-methyl-1-nitro-9,10-anthracenedione **M264**
 2-methyl-1-nitroanthraquinone **M264**
 2-methyl-4-nitrobenzenamine **M259**
 2-methyl-5-nitrobenzenamine **M260**
 4-methyl-3-nitrobenzenamine **M262**

N-methyl-4-nitrobenzenamine **M263**
 1-methyl-2-nitro-benzene **N179**
 1-methyl-3-nitrobenzene **N180**
 1-methyl-4-nitrobenzene **N181**
 2-methylnitrobenzene **N179**
 4-methylnitrobenzene **N181**
 4-methyl-2-nitrobenzeneamine **M261**
 2-methyl-5-nitroimidazole-1-ethanol **M327**
 6-[(1-methyl-4-1-nitro-5-1-imidazolyl)-mercaptapurine
A261
 6-(methyl-*p*-nitro-5-imidazolyl)-thiopurine **A261**
 6-[(1-methyl-4-nitro-1*H*-imidazol-5-yl)thio]-1*H*-purine
A261
 6-[(1-methyl-4-nitroimidazol-5-yl)thio]purine **A261**
N-methyl-*N*-nitromethanamine **D443**
 1-methyl-3-nitro-1-nitrosoguanidine **M265**
N-methyl-*N'*-nitro-*N*-nitrosoguanidine **M265**
 2-methyl-5-nitrophenol **N106**
 2-methyl-6-nitrophenol **N108**
 3-methyl-2-nitrophenol **N103**
 3-methyl-4-nitrophenol **N105**
 4-methyl-2-nitrophenol **N104**
 5-methyl-2-nitrophenol **N107**
 5-methyl-4-nitrophenol **N105**
 6-methyl-2-nitrophenol **N108**
 methyl *p*-nitrophenyl ketone **N73**
 methylnitropropyl-4-nitrosoaniline **M266**
N-(2-methyl-2-nitropropyl)-4-nitrosoaniline **M266**
N-(2-methyl-2-nitropropyl)-*p*-nitroso-aniline **M266**
N-(2-methyl-2-nitropropyl)-4-nitroso-benzenamine **M266**
 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone **N189**
 4-(*N*-methyl-*N*-nitrosoamino)-1-(3-pyridyl)-1-butanone
N189
N-methyl-*N*-nitrosoaniline **N160**
N-methyl-*N*-nitrosobenzamide **M267**
N-methyl-*N*-nitrosobenzenamine **N160**
N-methyl-*N*-nitrosobenzeneethanamine **N171**
N-(*N*-methyl-*N*-nitrosocarbamoyl)-*L*-ornithine **M268**
N-methyl-*N*-nitrosoethylamine **N161**
N-methyl-*N*-nitroso(ethyl carbamate) **N164**
N-methyl-*N*-nitrosoglycine **N175**
N-methyl-*N*-nitrosomethanamine **D444**
N-methyl-*N*-nitroso-*p*-toluenesulfonamide **M269**
N-methyl-*N*-nitroso-1-undecanamine **N162**
 1-methyl-1-nitroso-urea **N163**
N-methyl-*N*-nitrosourethane **N164**
N-methyl-*N*-nitrosovinylamine **N165**
 methyl nonyl ketone **U6**
 methyl *cis*-9-octadecenoate **M270**
 methylol **M116**
N-methylolchloracetamide **C204**
N-methylol-2-chloroacetamide **C204**
Z-methyl oleate **M270**
 Methyl Orange **M271**
 methyl orthoformate **T313**
 methyl orthosilicate **T91**
 4-methyl-2-oxetanone **B287**

methyloxirane **P330**
 methyl oxirane, polymer with oxirane **P218**
N-[(3-methyl-1-oxobutyl)-*L*-valyl-*L*-valyl-4-amino-3-
 hydroxy-6-methylheptanoyl-*L*-alanyl]-4-amino-3-
 hydroxy-6-methylheptanoic acid **P50**
 methyl 3-oxobutyrate **M152**
 2-methyl-6-oxo-2-heptene **M232**
 (Z)-(S)-2-methyl-4-oxo-3-(penta-2,4-dienyl)cyclopent-2-enyl
 (1*R*)-*trans*-2,2-dimethyl-3-(2-methylprop-1-
 enyl)cyclopropanecarboxylate **P352**
 (Z)-(S)-2-methyl-4-oxo-3-(penta-2,4-dienyl)cyclopent-2-enyl
 (E)-(1*R*)-*trans*-3-(2-methoxycarbonylprop-1-enyl)-2,2-
 dimethylcyclopropanecarboxylate **P353**
 S-2-methyl-oxo-3-(2-propynyl)-2-cyclopenten-1-yl 2,2-
 dimethyl-3-(2-methyl-1-propenyl)cyclopropane-
 carboxylate **P267**
 S-2-methyl-4-oxo-prop-2-ynylcyclopent-2-enyl (1*R*)-*cis*-
trans-2,2-dimethyl-3-(2-methylprop-1-enyl)cyclo-
 propanecarboxylate **P267**
 methylparaben **M272**
 8-methylparacymene **B278**
 Methyl Parasept **M272**
 methyl pentachlorophenate **P26**
 methyl pentachlorophenyl ether **P26**
 2-methylpentanal **M316**
 4-methyl-2-pentanamine **D404**
 2-methylpentane **M273**
 3-methylpentane **M274**
 2-methyl-2,4-pentanediol **M275**
 2-methylpentane-2,4-diol **M275**
 3-methyl-2,4-pentanedione **M276**
 2-methyl-1-pentanol **M277**
 2-methyl-3-pentanol **M278**
 3-methyl-3-pentanol **M279**
 4-methyl-1-pentanol **M280**
 4-methyl-2-pentanol **M281**
 4-methyl-2-pentanol, acetate **H77**
 2-methylpentanol-2-ol-4-one **D65**
 4-methyl-2-pentanone **M241**
 2-methylpentene **M282**
 2-methyl-1-pentene **M282**
 2-methylpent-1-ene **M282**
 2-methylpent-2-ene **M283**
 2-methyl-2-pentene **M283**
 4-methyl-1-pentene **M284**
 4-methylpent-1-ene **M284**
 4-methyl-2-pentene **M285**
 4-methylpent-2-ene **M285**
 4-methylpent-3-en-2-one **M91**
 3-methyl-2-(2-pentenyl)-(Z)-2-cyclopenten-1-one **J3**
 2-methylpent-1-ol **M277**
 4-methyl-2-pentyl acetate **H77**
 methyl pentyl ketone **H23**
 5-methyl-2-pentylphenol **A199**
 DL- α -methylphenethylamine **A193**
 methylphenol **C456**
 2-methylphenol **C458**

3-methylphenol **C457**
p-methylphenol **C459**
 4-methylphenol methyl ether **M157**
 α -methyl-3-phenoxybenzeneacetic acid **F13**
 [(methylphenoxy)methyl]oxirane **C460**
 2-[(2-methylphenoxy)methyl]oxirane **C461**
 [(4-methylphenoxy)methyl]oxirane **C462**
 methyl phenylacetate **M286**
 methyl-*N*-phenylacetyl-*N*-2,6-xylyl-DL-alaninate **B26**
 methylphenylamine **M156**
 1-[(2-methylphenyl)azo]-2-naphthalenol **O27**
 methylphenyl carbinol **P68**
 methylphenyldichlorosilane **D224**
 2-methyl-*m*-phenylenediamine **D90**
 2-methyl-*p*-phenylenediamine **D88**
 3-methyl-*o*-phenylenediamine **D86**
 4-methyl-*m*-phenylenediamine **D87**
 4-methyl-*o*-phenylenediamine **D92**
 2-methyl-*p*-phenylenediamine sulfate **D89**
 4-methyl-*m*-phenylene diisocyanate **T176**
 methylphenylene isocyanate **T175**
 methyl phenylethanoate **M286**
 1-(4-methylphenyl)ethanol **D402**
 methyl phenyl ether **A216**
 methylphenylethyl nitrosamine **N171**
N-(1-methyl-2-phenylethyl)- γ -phenylbenzenepropanamine **P271**
 1-(1-methyl-1-phenylethyl)-3-*p*-tolylurea **D603**
 2-methyl-*N*-phenyl-3-furancarboxamide **F10**
 2-methylphenyl glycidyl ether **C461**
 1-methyl-6-phenyl-1*H*-imidazo[4,5-*b*]pyridin-2-amine **P144**
p-methylphenyl isocyanate **T192**
 methyl phenyl ketone **A21**
 3-methylphenyl *N*-methylcarbamate **M324**
 4-methylphenylmethylcarbinol **D402**
N'-(4-methylphenyl)-*N'*-(1-methyl-1-phenylethyl)urea **D603**
 methylphenyl nitrosamine **N160**
 2-methyl-2-phenylpropane **B247**
 3-methyl-1-phenyl-2-pyrazolin-5-one **P121**
p-methylphenylsulfonic acid **T179**
p-methylphenylsulfonyl chloride **T180**
 (2-methylphenyl)thiourea **T193**
 1-methyl-3-phenyl-5-(3-trifluoromethylphenyl)-4(1*H*)-pyridinone **F86**
 (\pm)-*N*-methyl-3-phenyl-3-[(α,α,α -trifluoro-*p*-tolyl(oxy))-propylamine hydrochloride **F82**
 1-methyl-3-phenyl-5-(α,α,α -trifluoro-*m*-tolyl)-4-pyridone **F86**
 methyl phosphate **T324**
 methyl phosphite **T325**
 methylphosphonic dichloride **M287**
 methylphosphonofluoridic acid, 1-methylethyl ester **S8**
 methylphosphonoethioic acid, *O*-(*p*-nitrophenyl) *O*-phenyl ester **N137**
 methyl phosphoramidothioate **M111**
 methyl phthalate **D450**
 methylphytylnaphthochinonum **P181**
 2-methyl-3-phytyl-1,4-naphthoquinone **P181**
 3-[[[(4-methyl-1-piperazinyl)imino]methyl]rifamycin **R15**
 1-methylpiperidine **M288**
N-methylpiperidine **M288**
S-2-methylpiperidinocarbonylmethyl *O,O*-dipropyl phosphorodithioate **P205**
S-[2-(2-methyl-1-piperidinyl)-2-oxoethyl] *O,O*-dipropyl phosphorodithioate **P205**
 methyl polysiloxane **D373**
 6-methyl- $\Delta^{4,6}$ -pregnadien-17 α -ol-3,20-dione acetate **M44**
 methylpropanal **I97**
 2-methylpropanal **I97**
 2-methyl-1-propanamine **I89**
 2-methylpropane **I84**
 2-methylpropanitrile **I99**
 methyl propanoate **M290**
 2-methylpropanoic acid **I98**
 2-methylpropanoic acid, 2,2-dimethyl-1-(1-methylethyl)-1,3-propanediyl ester **T316**
 2-methylpropanoic acid, methyl ester **M242**
 2-methylpropanoic acid, 2-methylpropyl ester **I91**
 2-methyl-1-propanol **I85**
 2-methylpropan-2-ol **B214**
 2-methylpropenal **M103**
 2-methyl-2-propenal **M103**
 2-methylpropenamide **M105**
 2-methyl-2-propenamide **M105**
 2-methylpropene **I86**
 2-methylpropenenitrile **M108**
 methyl prop-2-enoate **M153**
 methyl 2-propenoate **M153**
 2-methyl-2-propenoate-2-ethyl-2-hydroxymethyl-1,3-propanediol trimethacrylate **T312**
 2-methylpropenoic acid **M106**
 2-methyl-2-propenoic acid **M106**
 2-methyl-2-propenoic acid anhydride **M107**
 2-methyl-2-propenoic acid, 2-hydroxypropyl ester **H117**
 2-methyl-2-propenoic acid, 2-methylpropyl ester **I92**
 1-methylpropenol **B220**
 2-methyl-2-propen-1-ol **M289**
 2-methyl-2-propenyl chloride **M109**
 methyl 1-propenyl ketone **P44**
 β -methylpropiolactone **B287**
 2-methylpropionaldehyde **I97**
 methyl propionate **M290**
 2-methylpropionic acid **I98**
 2-(2-methylpropoxy)naphthalene **I94**
 1-methylpropyl acetate **B234**
 2-methylpropyl acetate **I87**
 2-methylpropyl acetic acid ester **I87**
 2-methylpropyl alcohol **I85**
 1-methylpropylamine **B240**
 2-methylpropylamine **I89**
 methyl propylate **M290**
 methylpropylbenzene **C537**
N-(2-methylpropyl)-2-butanamine **D142**

2-(1-methylpropyl)-4,6-dinitrophenol **D510**
 2-(1-methylpropyl)-4,6-dinitrophenyl acetate **D511**
 2-(1-methyl-2-propyl)-4,6-dinitrophenyl isopropyl carbonate **D504**
 2-(1-methylpropyl)-4,6-dinitrophenyl-3-methyl-2-butenolate **B111**
 β -methylpropyl ethanoate **I87**
 2-methyl-2-propylethanol **M277**
 1-methyl-1-propylethene **M282**
 methyl propyl ether **M291**
 2-methylpropyl formate **I90**
 1-methylpropylidenebis[(1,1-dimethylethyl) peroxide] **D151**
 2-methylpropyl isobutyrate **I91**
 methyl propyl ketone **M292**
 2-methylpropyl methacrylate **I92**
 2-methylpropyl methyl ketone **M241**
N-(1-methylpropyl)-*N*-nitroso-2-butanamine **N147**
N-(1-methylpropyl)-*N*-nitroso-*sec*-butylamine **N147**
 2-(1-methylpropyl)phenol **B275**
 2-(1-methylpropyl) phenylmethylcarbamate **F12**
 2-methyl-2-propyl-1,3-propanediol dicarbamate **M57**
 2-methylpropyl propanoate **I95**
 2-methylpropyl propanoic acid ester **I95**
 2-methylpropyl 2-propenoic acid ester **I88**
 2-methylpropyl propinoate **I95**
 1-methylprop-2-ynyl 3-chlorocarbanilate **C117**
 1-methylprop-2-ynyl 3-chlorophenylcarbamate **C117**
 1-methyl-2-propynyl (3-chlorophenyl)carbamate **C117**
 methyl protocatechuic aldehyde **V17**
 2-methylpyrazine **M293**
 1-methylpyrene **M294**
 2-methylpyrene **M295**
 4-methylpyrene **M296**
 2-methylpyridine **P183**
 3-methylpyridine **P184**
 4-methylpyridine **P185**
 α -methylpyridine **P183**
 β -methylpyridine **P184**
 γ -methylpyridine **P185**
N-methyl-3-pyridinecarboxamide **M297**
 1-methyl-5*H*-pyrido[4,3-*b*]indol-3-amine **T365**
 1-methyl-9*H*-pyrido[3,4-*b*]indole **H6**
 5-methyl-2,4-(1*H*,3-*H*)-pyrimidinedione **T153**
 1-methyl-2-pyrrolidinone **M298**
 3-(*N*-methylpyrrolidino)pyridine **N54**
 3-(1-methyl-2-pyrrolidinyl)pyridine **N54**
 (5*S*)-3-(1-methyl-2-pyrrolidinyl)pyridine sulfate (2:1) **N55**
 1-methylpyrrolidone **M298**
N-methylpyrrolidone **M298**
 2-methylquinoline **Q4**
 4-methylquinoline **M299**
 5-methylquinoline **M300**
 6-methylquinoline **M301**
 7-methylquinoline **M302**
 8-methylquinoline **M303**
 γ -methylquinoline **M299**

p-methylquinoline **M301**
 Methyl Red **M304**
 methyl rhodanate **M310**
 methyl salicylate **M305**
 methyl silicone **P222**
 methylstyrene **M306**
 α -methylstyrene **M307**
ar-methylstyrene **M306**
 α -methylstyrol **M307**
 5-methyl-3-sulfanilamidoisoxazole **S136**
 methyl sulfanilylcarbamate **A251**
 methyl sulfate **D455**
 methyl sulphydrate **M115**
 methyl sulfide **D456**
 methylsulfinylmethane **D458**
 methyl sulfocyanate **M310**
 methyl sulfone **D457**
 methylsulfonic acid **M113**
 3-(methylsulfonyl)-2-butanone-*O*-[(methylamino)-carbonyl]oxime **B225**
 4-(methylsulfonyl)-2,6-dinitro-*N,N*-dipropylaniline **N64**
 4-(methylsulfonyl)-2,6-dinitro-*N,N*-dipropylbenzenamine **N64**
 methylsulfonylmethane **D457**
 2-methylsulfonyl-*O*-(*N*-methyl-carbamoyl)-butanon-(3)-oxime **B225**
 methyl sulfoxide **D458**
 methyl 2,3,5,6-tetrachloro-4-pyridyl sulfone **T52**
 2-methyltetrahydrofuran **M308**
 2-methyl-2-[4-(1,2,3,4-tetrahydro-1-naphthalenyl)phenoxy]-propanoic acid **N2**
 2-methyl-2-[*p*-(1,2,3,4-tetrahydro-1-naphthyl)phenoxy]-propanoic acid **N2**
 [*R*-(*R**,*R**-(*E*))-2-methyl-3-(3,7,11,15-tetramethyl-2-hexadecenyl)-1,4-naphthalenedione **P181**
N-methyl-*N*,2,4,6-tetranitrobenzenamine **N65**
 methyltheobromine **C20**
 2-(methylthio)benzothiazole **M309**
 3-(methylthio)-2-butanone-*O*-[(methylamino)-carbonyl]oxime **B223**
 3-(methylthio)butanone-*O*-methylcarbamoyloxime **B223**
 4-(methylthio)-*m*-cresol **M254**
 methyl thiocyanate **M310**
 methyl thioglycolate **M248**
 methylthiomethane **D456**
 3-(methylthio)-*O*-(methylamino)carbonyl]oxime-2-butanone **B223**
 methylthiophanate **T138**
 4-(methylthio)phenyl dimethyl phosphate **M311**
 methylthiophos **P14**
 6-methyl-2-thiouracil **M312**
 4-(methylthio)-3,5-xyleneol **D431**
 methyltoluene **X8**
 2-methyltoluene **X6**
 3-methyltoluene **X5**
 4-methyltoluene **X7**

m-methyltoluene **X5**
o-methyltoluene **X6**
p-methyltoluene **X7**
methyl toluene-4-sulfonate **M313**
methyl *p*-toluenesulfonate **M313**
2-methyl-*p*-toluidine **D396**
5-methyl-*o*-toluidine **D397**
methyl-*p*-tolylcarbinol **D402**
methyltopsin **T138**
methyl *p*-tosylate **M313**
5-methyl-1,2,4-triazolo[3,4*b*]benzothiazole **T272**
5-methyl-1,2,4-triazolo[3,4*b*][1,3]benzothiazole **T272**
methyl trichloride **C201**
methyltrichloromethane **T247**
methyl 2,4,6-trichlorophenyl ether **T239**
methyltrichlorosilane **M314**
6-methyl-1,3,8-trihydroxyanthraquinone **E18**
1-methyltrimethylene diacrylate **B206**
2-methyl-1,3,5-trinitrobenzene **T331**
Methyl Tuads **T147**
methylumbelliferone **M133**
5-methyluracil **T153**
methyllurea **M315**
1-methyllurea **M315**
N-methyllurea **M315**
methyllurethane **M184**
2-methylvaleraldehyde **M316**
2-methylvaleric aldehyde **M316**
1-methylvinyl acetate **I118**
methyl vinyl carbinol **B220**
methyl vinyl ether **M317**
methyl vinyl ketone **M318**
methylvinyl nitrosamine **N165**
2-methyl-5-vinylpyridine **M319**
methyl viologen(2+) **P11**
N-methyl-*N'*-2,4-xylyl-*N*-(*N*-2,4-xylylformimidoyl)-formamidine **A158**
Methyl Yellow **M320**
methyl zimate **Z19**
methyl zineb **P307**
methyrimol **D375**
Meticlor **C314**
meticlorpindol **C363**
metiram **M321**
Metmercaptopur **M123**
Metnilen **O41**
metobromuron **M322**
metolachlor **M323**
metolcarb **M324**
Metolquizalone **M119**
Metopryl **M291**
Metox **O57**
metoxuron **M325**
metribuzin **M326**
Metrifonate **T225**
Metron **P14**
metronidazole **M327**
metsulfuron-methyl **M328**
Meturon 4L **F47**
metyrapone **M329**
mevinphos **M330**
mexacarbate **M331**
Mezapur **M120**
Mezene **Z19**
mezineb **P307**
Mezotox **N112**
MFA (multifunctional acrylate) **T311**
MFH **M227**
MFM (multifunctional monomer) **T311**
MFP sodium **D563**
MH **M14**
MIA **I42**
Miazole **I9**
MIB **M240**
MIBC **M281**
MIBK **M241**
MIC **M243**
3-MIC **M281**
Michler's base **M212**
Michler's ketone **B128**
Michler's methane **M212**
miconazole **M332**
Microbator PC-78 **C136**
Micro-Cel **C43**
Micromet **S69**
microthene **P224**
Microvit A **V40**
Microx **Z12**
Midstream **D560**
Miedzian **C441**
Mil-Col **D600**
Milcurb **E70**
Milcurb **D375**
Mildin **F97**
Milgo:PP149 **E70**
Milk acid **L1**
Milogard **P302**
Milo-Pro **P302**
Milstem **E70**
Miltown **M57**
Minacide **P286**
mineral carbon **G45**
mineral naphtha **B47**
mineral oil **M333**
mineral pitch **A249**
Min-U-Lil **Q1**
minor components are polychloro-2-aminodiphenyl (PADs), such as 2',3,4,4',5-pentachloro-2-aminodiphenyl ether **E188**
Miocurin **G47**
miotisal **P10**
MIPA **A148**
MIPC **I116**
MIPCIN **I116**

MIPSIN **I116**
 Miral **I79**
 Mirapront **P88**
 mirbane oil **N82**
 mirex **M334**
 misonidazole **M335**
 Missile **P350**
 Mistral **F20**
 Mitac **A158**
 Mitacid **C535**
 Mitifon **T63**
 mitin N **F42**
 mitomycin **M336**
 mitomycin C **M336**
 Mitsui Blue B Base **D95**
 mixed xylenes **X8**
 Mixor **D464**
 mixture of *p*-methenols **T35**
 MJ 505 **P140**
 MK-23 **F67**
 MME **M252**
 MMH **M234**
 MMS **M253**
 MMT **M25**
 MMTP **M254**
 MNA **N160**
 MNB **M267**
 MNNG **M265**
 MNPA **N29**
 MNU **N163**
 MNUM **N164**
 MOCA **M210**
 Mocap **E74**
 Modur MRS **P114**
 Mogadon **N67**
 Mohr's Salt **I67**
 moldison **M11**
 molecular chlorine **C135**
 molecular hydrogen **H96**
 molecular oxygen **O60**
 molate **M337**
 molybdena **M339**
 molybdenum **M338**
 molybdenum(vi) oxide **M339**
 molybdenum trioxide **M339**
 molybdic acid anhydride **M339**
 molybdic anhydride **M339**
 MON-0573 **G40**
 monalide **M340**
 Monastral Blue BF **P176**
 Moncut **F92**
 Mondur P **P113**
 Monitan **P230**
 Monitor **M111**
 Monitox **V23**
 monoallylamine **A74**
 monoammonium sulfamate **A184**
 monoamylamine **P47**
 monoamyl phthalate **M347**
 monobasic lead acetate **L29**
 monobromoacetic acid **B158**
 mono-*n*-butylamine **B239**
 mono-*tert*-butylhydroquinone dimethyl ether **B256**
 monobutyl phthalate **M341**
 mono-*n*-butyl phthalate **M341**
 monocalcium arsenite **C23**
 monochloramide **C112**
 monochloramine **C112**
 monochloroacetaldehyde **C143**
 monochloroacetic acid **C145**
 monochloroacetic acid, ethyl ester **E106**
 monochloroacetic acid, methyl ester **M186**
 monochloroacetone **C146**
 monochloroacetyl chloride **C151**
 monochloroammonia **C112**
 monochlorobenzene **C163**
 1-monochlorodibenzo-*p*-dioxin **D107**
 monochlorodibenzofuran **D112**
 monochlorodifluoromethane **C192**
 monochloroethane **C196**
 monochloroethanoic acid **C145**
 2-monochloroethanol **C197**
 monochloroethylene **V30**
 α -monochlorohydrin **C265**
 monochloromethyl ether **B123**
 monochloropentafluoroethane **C234**
 monochlorosulfuric acid **C285**
 monochromium trioxide **C337**
 monocobalt oxide **C376**
 Monocron 9491 **I50**
 monocrotalin **M342**
 monocrotaline **M342**
 monocrotophos **M343**
 monoethanolamine **E62**
 monoethyl adipate **E136**
 monoethylamine **E90**
 monoethyl hexanedioate **E136**
 mono(2-ethylhexyl) phthalate **M344**
 monoethyl phosphonate, aluminium salt **F108**
 monoethylsulfuric acid **E173**
 monofluoroacetic acid **F55**
 monofluoroethane **F64**
 monofluoroethylene **V33**
 monofluorosulfuric acid **F75**
 monofluorotrichloromethane **F78**
 monofurfurylideneacetone **F129**
 Monogen Y100 **S76**
 monogermane **G13**
 monoglycol salicylate **G38**
 monoglyme **D381**
 monohydrated selenium dioxide **S13**
 monohydrochloride **P109**
 8-monohydromirex **P169**
 monoiodoacetic acid **I42**

monoiodoethane **I49**
 monoisobutylamine **I89**
 monoisopropanolamine **A148**
 monolinuron **M345**
 Monolite GT **D96**
 monomethylacetamide **M150**
 monomethylamine **M154**
 monomethylaminoethanol **M155**
 monomethylaniline **M156**
 monomethyldichlorosilane **D225**
 monomethylformamide **M225**
 monomethylhydrazine **M234**
 monomethylolacrylamide **H113**
 mononitrogen monoxide **N69**
 monononylphenol **N198**
 monooctyl phthalate **M346**
 mono-*n*-octyltin trichloride **O24**
 monopentadecylamine **P33**
 monopentyl phthalate **M347**
 mono-*n*-pentyl phthalate **M347**
 monophenylhydrazine **P108**
 monopotassium arsenate **P238**
 monopotassium dihydrogen arsenate **P238**
 monopropylamine **P323**
 monopropylene glycol **P327**
 monopropylene glycol methyl ether **M147**
 monopropylene glycol methyl ether **M146**
 monopyrrole **P366**
 Monorotox **M345**
 monosilane **S28**
 monosodium acid methanearsonate **M355**
 monosodium L-ascorbate **S46**
 monosodium sulfite **S48**
 mono-tertiarybutylhydroquinone **B262**
 mono[*p*-(1,1,3,3-tetramethylbutyl)phenyl]ether
 polyethylene glycol **O20**
 monothioethylene glycol **M62**
 monothiuram **M348**
 monotrithlorethylidene- α -D-glucose **C109**
 Monterey Kryocide **C472**
 montmorillonite **M349**
 monuron **M350**
 monuron-TCA **M351**
 Moracap **E68**
 Morflex 150 **D268**
 Morflex 210 **D519**
 Morflex 310 **D514**
 Morpan T **M364**
 Morphactin **C129**
 Morphia **M352**
 5 α ,6 α -morphinan **E151**
 morphinan-6-ol, 4,5-epoxy-3-methoxy-17-methyl-, (5 α ,6 α)-
 D344
 morphine **M352**
 (-)-morphine **M352**
 Morphium **M352**
 morpholine **M353**
 5-(morpholinomethyl)-3-[(5-nitrofurfurylidene)amino]-2-
 oxazolidinone **F122**
 1,5-(morpholinomethyl)-3-[(5-nitrofurfurylidene)amino]-2-
 oxazolidinone hydrochloride **O49**
 5-(morpholinomethyl)-3-[(5-nitrofurfurylidene)amino]-2-
 oxazolidinone, monohydrochloride **O49**
 morpholinophosphonic acid, dimethyl ester **D432**
 5-(4-morpholinylmethyl)-3-[[[(5-nitro-2-furanyl)methylene]-
 amino]-(S)-2-oxazolidine, monohydrochloride **O49**
 4-morpholinylphosphonic acid, dimethyl ester **D432**
 morphothion **M354**
 Morphotox **M354**
 Morpolose M400 **M185**
 Morsodren **M251**
 Morta-Lok **C37**
 Morton Soil Drench **M251**
 Moryl **C60**
 moth flakes **N9**
 Motrin **I2**
 Mountain Green **P15**
 Mouser **B150**
 Moxisylte **T155**
 MPCM **X16**
 MPP **F24**
 MPT **V41**
 M-pyrol **M298**
 MS 1053 **M37**
 MSF **M114**
 MSL **S64**
 MSMA **M355**
 MTBE **M181**
 MTBHQ **B262**
 M & T Chemicals 1222-45 **T327**
 MTMC **M324**
 MTO-460 **P150**
 MTU **M312**
 Mucap **E74**
 Muccira **K3**
 Mucodyne **C67**
 Mucopront **C67**
 Multiphos **M111**
 Multiprop **C129**
 Murfotox **M37**
 muriate of platinum **P213**
 muriate of potash **P243**
 muriate of potassium **P243**
 muriatic acid **H99**
 muriatic ether **C196**
 Muritan **C323**
 Murox **N209**
 Murphotox **M37**
 Murvis **F22**
 muscimol **M356**
 Musculamine **S107**
 musk ambrette (synthetic) **M357**
 musk xylene **M358**
 musk xylol **M358**

Musol **P132**
 mustard gas **M359**
 Mustargen **M38**
 Muster **E57**
 Mustine **M38**
 Mutamycin **M336**
 Muthmann's liquid **T40**
 MXDA **X17**
 Myacyne **N34**
 Mycelex **C365**
 myclobutanil **M360**
 Myco **F97**
 mycoin **P16**
 Mycostatin **N210**
 mycotoxin F2 **Z1**
 Mycristadin **N34**
 Myleran **B195**
 Myobid **P5**
 Myocaine **G47**
 Myofer **I70**
 Myprozine **P191**
 myrcene **M361**
 β -myrcene **M361**
 myristaldehyde **M363**
 myristic acid **M362**
 myristic aldehyde **M363**
 myristyl aldehyde **M363**
 myristyltrimethylammonium bromide **M364**
 myrtenal **M365**
 myrticlorin **R22**
 Mysoline **P272**
 Mytab **M364**
 Mytrol **F44**
 N-2790 **F99**
 NAAM **N21**
 Nabac **H41**
 nabam **N1**
 Nacco **I25**
 Nacconate 100 **T176**
 Nacconate H12 **M211**
 Nacid **H108**
 Nacid **N4**
 Nacol 16-98 **C102**
 Nacol 6-98 **H65**
 Na DMDC **S64**
 Nadone **C509**
 nafenopin **N2**
 β -naftol **N18**
 Nafusaku **N22**
 Naja **F21**
 Nakar **B30**
 Nalcrom **S57**
 naled **N3**
 Nalfon (calcium salt) **F13**
 nalidixic acid **N4**
 nalidixinic acid **N4**
 Nalix **N4**
 Nalkylene 500 **P100**
 5-NAN **N71**
 Nansa EVM 70/B **C32**
 Nansa HS80 **S65**
 naphtha **N5**
 naphthacene **N6**
 naphthacenecarboxamide **C316**
 2-naphthacenecarboxamide, 4-(dimethylamino)-
 1,4,4a,5,5a,6,11,12a-octahydro-3,5,6,10,12,12a-
 hexahydroxy-6-methyl-1,11-dioxo-, [4S-
 (4 α ,4a α ,5 α ,5a α ,6 β ,12a α)]- **O64**
 α -naphthal **N7**
 1-naphthaldehyde **N7**
 2-naphthaldehyde **N8**
 α -naphthaldehyde **N7**
 β -naphthaldehyde **N8**
 1-naphthalenamine **N23**
 2-naphthalenamine **N24**
 naphthalene **N9**
 1-naphthaleneacetamide **N21**
 1-naphthaleneacetic acid **N22**
 1-naphthalenecarboxaldehyde **N7**
 2-naphthalenecarboxaldehyde **N8**
 naphthalene- α -carboxylic acid **N15**
 1-naphthalenecarboxylic acid **N15**
 2-naphthalenecarboxylic acid **N16**
 2-naphthalenecarboxylic acid, 5-[(chloro-4-methyl-2-
 sulfophenyl)azo]-3-hydroxy-, calcium salt **C418**
 naphthalenecarboxylic acid, cobalt salt **C375**
 1,5-naphthalenediamine **N10**
 naphthalene 1,5-diisocyanate **N11**
 naphthalene, 1,5-dimethyl- **D436**
 1,4-naphthalenedione **N20**
 2,7-naphthalenedisulfonic acid, 3,3'-[[1,1'-biphenyl]-4,4'-
 diylbis(azo)]bis(5-amino-4-hydroxy)-, tetrasodium salt **C404**
 2,7-naphthalenedisulfonic acid, 3,3'-((3,3'-dimethoxy-4,4'-
 biphenylene)bis(azo))bis(5-amino-4-hydroxy)-,
 tetrasodium salt **C405**
 1,3-naphthalenedisulfonic acid, 8-[(3,3'-dimethyl-4'-[(4-
 methylphenyl)sulfonyl]oxy]phenyl]azo][1,1'-biphenyl]-
 4-yl]azo]-7-hydroxy-, disodium salt **C398**
 1,3-naphthalenedisulfonic acid, 8-[[4'-[(4-
 ethoxyphenyl)azo]-3,3'-dimethyl[1,1'-biphenyl]-4-
 yl]azo]-7-hydroxy-, disodium salt **C408**
 1,3-naphthalenedisulfonic acid, 7-hydroxy-8-(phenylazo)-,
 disodium salt **C392**
 Naphthalene Ink Scarlet 4R **C394**
 naphthalene oil **C453**
 2-naphthalenesulfonic acid, compound with [S-(R*,S*)]-3-
 (dimethylamino)-2-methyl-1-phenyl-1-(phenylmethyl)-
 propyl propanoate (1:1) **P320**
 1-naphthalenesulfonic acid, 4-hydroxy-3-[(4-sulfonyl-1-
 naphthalenyl)azo]-, disodium salt **C393**
 1-naphthalenol **N17**
 2-naphthalenol **N18**
 2-naphthalenol, 1-[(4-methyl-2-nitrophenyl)azo]- **C416**

2-[(1-naphthalenylamino)carbonyl]benzoic acid **N30**
N-1-naphthalenyl-1,2-ethanediamine dihydrochloride **N25**
 1-naphthalenyl *N*-methylcarbamate **C63**
 2-naphthalenyloxyacetic acid **N26**
 naphthalidine **N23**
 naphthaline **N9**
 Naphthanil Blue B Base **D95**
 naphthanthracene **B43**
 $\delta^5,7,9$ -naphthantriene **T80**
 naphtha safety solvent **S119**
 naphthenic acid **N12**
 naphthenic acid, copper salt **C437**
 Naphthenil Red B Base **M141**
 1,4-naphthionic acid **A132**
 naphtho[1,2,3,4-*def*]chrysene **D115**
 α -naphthoflavone **N13**
 β -naphthoflavone **N14**
 α -naphthofluorene **B60**
 naphtho[2,1-*b*]furan-1,11(2*H*)-dione, 5,6,9,17,19,21-hexahydroxy-23-methoxy-2,4,12,16,18,20,22-heptamethyl-8-[*N*-(4-methyl-1-piperazinyl)formimidoyl]-2,7-(epoxypentadeca[1,11,13]trienimino)-, 21-acetate **R15**
 1-naphthoic acid **N15**
 2-naphthoic acid **N16**
 α -naphthoic acid **N15**
 β -naphthoic acid **N16**
 naphth-2-ol **N18**
 1-naphthol **N17**
 2-naphthol **N18**
 α -naphthol **N17**
 Naphthol AS **N19**
 Naphthol AS-A **N19**
 naphthol B **N18**
 1-naphthol-3,6-disulfonic acid, 2,2'-(4,4'-biphenylene-bisazo)bis(8-amino)-, tetrasodium salt **C404**
 1,4-naphthoquinone **N20**
 α -naphthoquinone **N20**
 naphtho[1,2-*b*]thianaphthene **B66**
 naphtho[2,1-*b*]thianaphthene **B65**
 naphtho[3,2-*b*]thianaphthene **B67**
 α -naphthothiurea **N27**
 2-naphthoxyacetic acid **N26**
 β -naphthoxyacetic acid **N26**
 2-(α -naphthoxy)-*N,N*-diethylpropionamide **N28**
 1-naphthylacetamide **N21**
 2-(1-naphthyl)acetamide **N21**
 1-naphthylacetic acid **N22**
 2-(1-naphthyl)acetic acid **N22**
 α -naphthylacetic acid **N22**
 β -naphthyl alcohol **N18**
 1-naphthylaldehyde **N7**
 α -naphthylaldehyde **N7**
 β -naphthylaldehyde **N8**
 1-naphthylamine **N23**
 2-naphthylamine **N24**
 α -naphthylamine **N23**

β -naphthylamine **N24**
 2-naphthylamine mustard **C142**
 1-naphthylamine-4-sulfonic acid **A132**
 1-naphthylamine-6-sulfonic acid **A133**
 1-naphthylamine-7-sulfonic acid **A136**
 2-naphthylamine-1-sulfonic acid **A131**
 2-naphthylamine-6-sulfonic acid **A134**
 2-naphthylamine-7-sulfonic acid **A135**
 β -naphthylamine-8-sulfonic acid **A135**
N-(2-naphthyl)aniline **P124**
 (β -naphthyl)benzene **P123**
 α -naphthylcarboxaldehyde **N7**
 β -naphthylcarboxaldehyde **N8**
 α -naphthylcarboxylic acid **N15**
 α -naphthyl chloride **C217**
 β -naphthyl chloride **C218**
 1,2-(1,8-naphthylene)benzene **F48**
 1,5-naphthylenediamine **N10**
N-(1-naphthyl)ethylenediamine dihydrochloride **N25**
 β -naphthyl hydroxide **N18**
 1-naphthyl *N*-methylcarbamate **C63**
 (2-naphthoxy)acetic acid **N26**
 α -naphthylphthalamic acid **N30**
N-1-naphthylphthalamic acid **N30**
 α -naphthylthiocarbamide **N27**
 1-naphthylthiourea **N27**
 1-(1-naphthyl)-2-thiourea **N27**
N-(1-naphthyl)thiourea **N27**
 napropamide **N28**
 naproxen **N29**
 naptalam **N30**
 Narcotane **H4**
 naryclen **A26**
 Nardelzine **P64**
 Nardil **P64**
 naringenin **N31**
 (2*S*)-naringenin **N31**
 (-)-naringenin **N31**
 (-)-(2*S*)-naringenin **N31**
 naringenine **N31**
 naringetol **N31**
 Natamycin **P191**
 natrium **S39**
 Natulan **I1**
 natural graphite **G45**
 natural lead sulfide **L31**
 natural pearl essence **G50**
 natural smithsonite **Z5**
 natural tartaric acid **T9**
 Natural Yellow 14 **E18**
 Naturchrom Turmeric **C478**
 Navadel **D531**
 Navchor **F8**
 Navron **F53**
 Naxel AAS-98S **D589**
 NC5016 **F5**
 NC8438 **E72**

NCI-C01876 **A112**
 NCI-C01923 **M264**
 NCI-C02006 **B128**
 NCI-C02551 **C11**
 NCI-C02813 **P204**
 NCI-C02993 **C454**
 NCI-C03281 **N25**
 NCI-C03521 **B78**
 NCI-C03554 **T50**
 NCI-C03736 **A209**
 NCI-C03850 **B75**
 NCI-C04615 **A78**
 NCI-C04728 **C546**
 NCI-C04864 **V24**
 NCI-C04922 **C548**
 NCI-C05258 **C476**
 NCI-C09007 **C465**
 NCI-C50011 **B64**
 NCI-C50373 **V28**
 NCI-C50737 **C547**
 NCI-C50748 **G53**
 NCI-C5099 **P330**
 NCI-C52459 **T49**
 NCI-C54842 **M16**
 NCI-C54897 **H8**
 NCI-C54999 **V31**
 NCI-C55005 **C509**
 NCI-C55072 **C122**
 NCI-C55594 **M184**
 NCI-C55845 **B74**
 NCI-C56166 **B61**
 NCI-C56348 **C351**
 NCI-C56393 **E97**
 NCI-C56440 **H45**
 NCI-C56519 **M61**
 NCI-C60399 **M64**
 NCI-C60979 **I102**
 NCI-C61 **B11**
 NCI-C61325 **C478**
 NCI-C61405 **H54**
 4NDB **N134**
 NDBA **N146**
 NDEA **N149**
 NDELA **N148**
 NDHU **N150**
 NDPA **N156**
 NDPA **N155**
 NEA **N157**
 Neamine **N35**
 Nebijn **F91**
 Nebramycin **N35**
 Nebulin **T14**
 neburon **N32**
 Neemix **A258**
 Negamicin **N35**
 Negram **N4**
 Neguron **T225**

NEM **E152**
 Nema **T51**
 NEMA **N161**
 Nemacur **F3**
 Nemafos **T135**
 Nemamort **D26**
 Nemazine **P83**
 Nemazyd **S47**
 Nembutal **P45**
 Nem-a-tak **F109**
 nendrin **E25**
 Neobis **D315**
 neocidol **D99**
 Neodorm **P45**
 neodymium **N33**
 Neo-Fat 12 **L8**
 Neo-Fat 18 **S112**
 Neoloid **C94**
 neomycin **N34**
 neomycin A **N35**
 neomycin B **N36**
 neomycin C **N37**
 neomycin E **N38**
 Neopec **F7**
 Neopelex 05 **S65**
 Neopellis **T122**
 neopentane **N39**
 neopentenediol **N40**
 neopentenediol diacrylate **N41**
 neopentylene glycol **N40**
 neopentyl glycol **N40**
 neopentyl glycol diacrylate **N41**
 Neoplatin **C350**
 Neo-Pyramin **T85**
 Neoron **B187**
 Neosar **C529**
 Neo Silox D **S54**
 Neosorb **S104**
 Neosorexa **D323**
 neo-testis **T38**
 Neothyl **M291**
 Neotopsin **T138**
 neovitamin A acid **I138**
 Neozone **P124**
 Neozopam **N67**
 Neporex **C545**
 neral **C351**
 Nesontil **O48**
 Nespor **M21**
 Nessler reagent **P266**
 Neuridine **S107**
 Neurocalm **T369**
 Neurotone **G47**
 neutral ammonium fluoride **A173**
 neutralised verdigris **C430**
 Neutralizer K-126 **S51**
 Neutralizer K-140 **S51**

Neutralizer K-938 **S51**
 neutral lead acetate **L12**
 Neutral Red **N42**
 neutral sodium chromate **S56**
 Neviken **C42**
 Nevirol **P130**
 New Coccine **C394**
 New Green **P15**
 NF-246 **N58**
 NFTA **N117**
 NHMI **N159**
 Niac **N57**
 niacin **N57**
 niacinamide **N53**
 Niagara 5943 **T202**
 Niagaramite **A232**
 Niagestin **M44**
 Niagorathal **E23**
 nialamide **N43**
 Nialate **E68**
 Nias 3CF **T350**
 Nicasir **N53**
 NIC-C56633 **T299**
 nickel **N44**
 nickel ammonium sulfate **N45**
 nickel carbonyl **N51**
 (T-4)-nickel carbonyl (Ni(CO)₄) **N51**
 nickel chloride **N46**
 nickel(II) chloride **N46**
 nickel chloride (NiCl₂) **N46**
 nickel dichloride **N46**
 nickel dihydroxide **N47**
 nickel hydroxide **N47**
 nickel(II) hydroxide **N47**
 nickel hydroxide (Ni(OH)₂) **N47**
 nickel monosulfate **N50**
 nickel nitrate **N48**
 nickelous chloride **N46**
 nickelous hydroxide **N47**
 nickelous sulfate **N50**
 nickel subsulfide **N49**
 nickel sulfate **N50**
 nickel(II) sulfate **N50**
 nickel sulfide (Ni₃S₂) **N49**
 nickel tetracarbonyl **N51**
 Niclofen **N112**
 niclosamide **N52**
 niclosamide, 2-hydroxyethylamine salt **C362**
 Nicocap **N57**
 nicotine **N54**
 nicotinamide **N53**
 nicotine **N54**
 L-nicotine **N54**
 nicotine acid tartrate **N56**
 nicotine bitartrate **N56**
 nicotine hydrogen tartrate **N56**
 nicotine sulfate **N55**

nicotine sulfate (2:1) **N55**
 nicotine tartrate **N56**
 nicotinic acid **N57**
 nicotinic acid amide **N53**
 nicotinic acid methylamide **M297**
 nicotinitrile **C488**
 Niflex **E85**
 nifuradene **N58**
 nifurthiazole **N59**
 Nigrosine **C385**
 Nikkol DID **D357**
 Nimitex **T19**
 Nimrod **B193**
 ningidrin **N60**
 ninhydrin **N60**
 niobe oil **M161**
 niobium **N61**
 Nipa **P332**
 Nipabutyl **B269**
 Nipacide BCP **B96**
 Nipacide MX **C306**
 Nipagallin **P332**
 Nipagin A **E158**
 Nipagin M **M272**
 Nipanox BHT **B245**
 NiPan S-20 Solvent **N139**
 Nipantiox 1-F **B244**
 Nipasol **P336**
 niridazole **N62**
 Niscolen **P218**
 Nissan Unilube DE60 **P218**
 niter **P257**
 nithiazide **N63**
 nitralin **N64**
 Nitraline **N64**
 nitramine **N65**
 nitrapyrin **N66**
 nitrazepam **N67**
 nitrazol I-AS **N19**
 nitric acid **N68**
 nitric acid, barium salt **B13**
 nitric acid, butyl ester **B268**
 nitric acid, caesium salt **C18**
 nitric acid, calcium salt **C36**
 nitric acid, chromium(3+) salt **C336**
 nitric acid, copper(2+) salt **C438**
 nitric acid, iron(3+) salt **I73**
 nitric acid, lead (2+) salt **L25**
 nitric acid, magnesium salt **M5**
 nitric acid, mercury(1+) salt **M77**
 nitric acid, mercury(2+) salt **M78**
 nitric acid, 1-methylethyl ester **I129**
 nitric acid, pentyl ester **A202**
 nitric acid, potassium salt **P257**
 nitric acid, propyl ester **P334**
 nitric acid, silver(1+) salt **S36**
 nitric acid, sodium salt **S80**

- p>nitric acid, strontium salt
- S123**
-
- nitric acid, thallium(I) salt
- T106**
-
- nitric anhydride
- D477**
-
- nitric oxide
- N69**
-
- nitrilotriacetic acid
- N70**
-
- nitrilotriethanol
- T276**
-
- 2,2',2''-nitrilotriethanol
- T276**
-
- 1,1',1''-nitrilotri-2-propanol
- T297**
-
- 5-nitroacenaphthene
- N71**
-
- 3-nitro-
- p*
- acetophenelide
- N72**
-
- 5-nitro-
- p*
- acetophenetidide
- N72**
-
- 4'-nitroacetophenone
- N73**
-
- p*
- nitroacetophenone
- N73**
-
- m*
- nitroaminobenzene
- N75**
-
- 2-nitro-4-aminophenol
- A140**
-
- 5-nitro-2-aminophenol
- A139**
-
- o*
- nitro-
- p*
- aminophenol
- A140**
-
- p*
- nitro-
- o*
- aminophenol
- A138**
-
- 5-nitro-2-aminothiazole
- A141**
-
- 2-nitroaniline
- N74**
-
- 3-nitroaniline
- N75**
-
- 4-nitroaniline
- N76**
-
- m*
- nitroaniline
- N75**
-
- o*
- nitroaniline
- N74**
-
- p*
- nitroaniline
- N76**
-
- 2-nitro-
- p*
- anisidine
- M143**
-
- 4-nitro-
- o*
- anisidine
- M141**
-
- 5-nitro-
- o*
- anisidine
- M142**
-
- 2-nitroanisole
- N77**
-
- 3-nitroanisole
- N78**
-
- 4-nitroanisole
- N79**
-
- m*
- nitroanisole
- N78**
-
- o*
- nitroanisole
- N77**
-
- p*
- nitroanisole
- N79**
-
- 4-nitroanthranilic acid
- N80**
-
- nitrobarite
- B13**
-
- 3-nitrobenzaldehyde
- N81**
-
- m*
- nitrobenzaldehyde
- N81**
-
- 3-nitrobenzenamine
- N75**
-
- nitrobenzene
- N82**
-
- nitrobenzene, 2-bromo-
- B180**
-
- nitrobenzene, 4-bromo-
- B181**
-
- m*
- nitrobenzenecarboxylic acid
- N88**
-
- p*
- nitrobenzenecarboxylic acid
- N89**
-
- 2-nitro-1,4-benzenediamine
- N133**
-
- 4-nitro-1,2-benzenediamine
- N134**
-
- 4-nitrobenzenemethanol
- N96**
-
- 2-nitrobenzenesulfonic acid
- N83**
-
- 3-nitrobenzenesulfonic acid
- N84**
-
- 4-nitrobenzenesulfonic acid
- N85**
-
- 5-nitro-1
- H*
- benzimidazole
- N86**
-
- 5(6)-nitrobenzimidazole
- N86**
-
- 2-nitrobenzoic acid
- N87**
-
- 3-nitrobenzoic acid
- N88**
-
- 4-nitrobenzoic acid
- N89**
-
- o*
- nitro-benzoic acid
- N87**
-
- nitrobenzol
- N82**
-
- 2-nitrobenzonitrile
- N90**
-
- 3-nitrobenzonitrile
- N91**
-
- 4-nitrobenzonitrile
- N92**
-
- 2-nitrobenzotrifluoride
- N93**
-
- 3-nitrobenzotrifluoride
- N94**
-
- 4-nitrobenzotrifluoride
- N95**
-
- 4-nitrobenzyl alcohol
- N96**
-
- p*
- nitrobenzyl alcohol
- N96**
-
- 4-nitrobenzyl chloride
- N97**
-
- p*
- nitrobenzyl chloride
- N97**
-
- 2-nitrobiphenyl
- N98**
-
- 2-nitro-1,1'-biphenyl
- N98**
-
- 3-nitrobiphenyl
- N99**
-
- 3-nitro-1,1'-biphenyl
- N99**
-
- 4-nitrobiphenyl
- N100**
-
- 4-nitro-1,1'-biphenyl
- N100**
-
- m*
- nitrobiphenyl
- N99**
-
- o*
- nitrobiphenyl
- N98**
-
- p*
- nitrobiphenyl
- N100**
-
- nitrobromoform
- T206**
-
- 1-nitrobutane
- N101**
-
- nitrocarbol
- N127**
-
- nitrocellulose
- C98**
-
- 4-nitro-2-chloroaniline
- C220**
-
- m*
- nitrochlorobenzene
- C223**
-
- o*
- nitrochlorobenzene
- C222**
-
- p*
- nitrochlorobenzene
- C224**
-
- 3-nitro-4-chlorobenzotrifluoride
- C225**
-
- 1-nitro-1-chloroethane
- C226**
-
- nitrochloroform
- C259**
-
- 2-nitro-4-chlorophenol
- C229**
-
- 2-nitro-5-chlorophenol
- C230**
-
- 4-nitro-3-chlorophenol
- C228**
-
- p*
- nitro-
- m*
- chlorophenyl dimethyl thionophosphate
- C320**
-
- 1-nitro-1-chloropropane
- C231**
-
- 2-nitro-6-chlorotoluene
- C233**
-
- 3-nitro-4-chloro-
- α,α,α
- trifluorotoluene
- C225**
-
- 6-nitrochrysene
- N102**
-
- nitrocotton
- C98**
-
- 2-nitro-
- m*
- cresol
- N103**
-
- 2-nitro-
- p*
- cresol
- N104**
-
- 4-nitro-
- m*
- cresol
- N105**
-
- 5-nitro-2-cresol
- N106**
-
- 5-nitro-
- o*
- cresol
- N106**
-
- 6-nitro-
- m*
- cresol
- N107**
-
- 6-nitro-
- o*
- cresol
- N108**
-
- o*
- nitrocresol
- N107**
-
- p*
- nitro-
- m*
- cresol
- N105**
-
- p*
- nitrocumene
- N109**
-
- nitrocyclohexane
- N110**
-
- 4-nitro-1,2-diaminobenzene
- N134**
-
- 4-nitro-1,3-dichlorobenzene
- D228**
-
- N*
- nitrodimethylamine
- D443**
-
- 1-nitro-2,4-dimethylbenzene
- N187**
-
- 2-nitro-1,3-dimethylbenzene
- N185**
-
- 4-nitro-1,2-dimethylbenzene
- N188**
-
- 4-nitro-1,3-dimethylbenzene
- N187**

2-nitrodiphenyl **N98**
 3-nitrodiphenyl **N99**
 4-nitrodiphenyl **N100**
 N-nitro DMA **D443**
 nitrodacrylic acid **N89**
 nitroethane **N111**
 Nitrofan N **D511**
 Nitro Fast Yellow SL **C427**
 nitrofen **N112**
 3-nitrofluoranthene **N113**
 2-nitrofluorene **N114**
 2-nitro-9H-fluorene **N114**
 5-nitro-2-furaldehyde semicarbazone **N116**
 nitrofurantoin **N115**
 1-[[[(5-nitro-2-furanyl)methylene]amino]-2,4-imidazolidinedione **N115**
 3-[[[(5-nitro-2-furanyl)methylene]amino]-2-oxazolinone **F126**
 α-[(5-nitro-2-furanyl)methylene]-2-furanacetamide **F132**
 2-[(5-nitro-2-furanyl)methylene]hydrazinecarboxamide **N116**
 2-[3-(5-nitro-2-furanyl)-1-[2-(5-nitro-2-furanyl)ethenyl]-2-propenylidene]hydrazinecarboximidamide **N184**
 5-(5-nitro-2-furanyl)-1,3,4-thiadiazol-2-amine **A137**
 2-[4-(5-nitro-2-furanyl)-2-thiazolyl] hydrazinecarboxaldehyde **N59**
 nitrofurazolidone **F126**
 nitrofurazolidonum **F126**
 nitrofurazone **N116**
 5-nitro-2-furfural semicarbazone **N116**
 1-[(5-nitro-2-furfurylidene)amino]hydantoin **N115**
 N-(5-nitrofurfurylidene)-1-amino-2-imidazolidinone **N58**
 1-[(5-nitrofurfurylidene)amino]-2-imidazolidinone N-[(5-nitro-2-furfurylideneamino)]-2-imidazolidinone **N58**
 3-[(5-nitrofurfurylidene)amino]-2-oxazolidinone **F126**
 (5-nitro-2-furfurylideneamino)urea **N116**
 2-(5-nitro-2-furyl)-5-amino-1,3,4-thiadiazole **A137**
 5-(5-nitro-2-furyl)-2-amino-1,3,4-thiadiazole **A137**
 [[3-(5-nitro-2-furyl)-1-[2-(5-nitro-2-furyl)vinyl]allylidene]-amino]guanidine **N184**
 N-[4-(5-nitro-2-furyl)-2-thiazolyl]acetamide **N117**
 N-[4-(5-nitro-2-furyl)-2-thiazolyl]formamide **N118**
 nitrogen **N119**
 nitrogen dioxide **N120**
 nitrogen fluoride **N121**
 nitrogen monoxide **N69**
 nitrogen mustard **M38**
 nitrogen mustard amine oxide **M39**
 nitrogen mustard oxide **M39**
 nitrogen mustard N-oxide **M39**
 nitrogen oxide **N183**
 nitrogen oxide (NO₂) **N120**
 nitrogen oxide (N₂O₃) **D479**
 nitrogen oxide (N₂O₄) **D478**
 nitrogen oxide (N₂O₅) **D477**
 nitrogen pentoxide **D477**
 nitrogen peroxide **N120**
 nitrogen tetroxide **D478**
 nitrogen trifluoride **N121**
 nitroglycerin **G26**
 nitroglycol **E115**
 nitroguanidine **N122**
 1-nitroguanidine **N122**
 α-nitroguanidine **N122**
 3-nitro-3-hexene **N123**
 2-nitro-2-(hydroxymethyl)-1,3-propanediol **T357**
 2-nitro-5-hydroxytoluene **N105**
 2-nitroimidazole **N124**
 2-nitro-1H-imidazole **N124**
 4-nitroimidazole **N125**
 4-nitro-1H-imidazole **N125**
 5-nitroindole **N126**
 5-nitro-1H-indole **N126**
 nitroisopropane **N139**
 4-nitroisopropylbenzene **N109**
 Nitrol **M266**
 nitrolime **C29**
 nitrol (pesticide) **N128**
 nitromethane **N127**
 3-nitro-6-methoxyaniline **M142**
 1-nitro-2-methylanthraquinone **M264**
 2-nitro-3-methyl phenol **N103**
 2-nitro-4-methylphenol **N104**
 4-nitro-3-methylphenol **N105**
 4-nitro-5-methylphenol **N105**
 5-nitro-2-methylphenol **N106**
 o-nitro-p-methylphenol **N104**
 p-nitro-m-methylphenol **N105**
 1-nitronaphthalene **N128**
 2-nitronaphthalene **N129**
 α-nitronaphthalene **N128**
 β-nitronaphthalene **N129**
 5-nitronaphthaleneethylene **N71**
 3-nitro-1-nitroso-1-propylguanidine **P335**
 N'-nitro-N-nitroso-N-propylguanidine **P335**
 nitropentachlorobenzene **Q12**
 Nitrophen **N112**
 2-nitrophenol **N130**
 3-nitrophenol **N131**
 4-nitrophenol **N132**
 m-nitrophenol **N131**
 o-nitrophenol **N130**
 p-nitrophenol **N132**
 1-(p-nitrophenoxy)-2,3-epoxypropane **G33**
 [(4-nitrophenoxy)methyl]oxirane **G33**
 1-(4-nitrophenoxy)-2,3-propylene oxide **G33**
 m-nitrophenylamine **N75**
 p-nitrophenylamine **N76**
 o-nitrophenyl bromide **B180**
 p-nitrophenyl bromide **B181**
 p-nitrophenyl diethyl phosphate **P10**
 2-nitro-1,4-phenylenediamine **N133**
 2-nitro-p-phenylenediamine **N133**
 4-nitro-1,2-phenylenediamine **N134**

4-nitro-*o*-phenylenediamine **N134**
 1-(4-nitrophenyl)-ethanone **N73**
 4-nitrophenyl glycidyl ether **G33**
 2-nitrophenylhydrazine **N135**
 4-nitrophenylhydrazine **N136**
o-nitrophenylhydrazine **N135**
p-nitrophenylhydrazine **N136**
 (4-nitrophenyl)methanol **N96**
 4-nitrophenyl methyl ether **N79**
o-nitrophenyl methyl ether **N77**
p-nitrophenyl methyl ketone **N73**
O-(4-nitrophenyl) *O*-phenyl methylphosphonothioate **N137**
 2-(*p*-nitrophenyl)propane **N109**
N-(4-nitrophenyl)-*N'*-(3-pyridinylmethyl)urea **P362**
 3-nitrophenylsulfonic acid **N84**
p-nitrophenylsulfonic acid **N85**
 1-nitropropane **N138**
 2-nitropropane **N139**
 β -nitropropane **N139**
 3-nitropropanoic acid **N140**
 3-nitropropionic acid **N140**
 β -nitropropionic acid **N140**
 1-nitropyrene **N141**
 2-nitropyrene **N142**
 3-nitropyrene **N141**
 4-nitropyrene **N143**
 4-nitropyridine 1-oxide **N144**
 4-nitropyridine *N*-oxide **N144**
 Nitrosan K **M207**
N-nitrosoazacyclooctane **N159**
 nitrosobaygon **N173**
N-nitrosobis(2-hydroxyethyl)amine **N148**
N-nitrosobis(2-hydroxypropyl)amine **N151**
N-nitrosobis(2,2,2-trifluoroethyl)amine **N145**
 1'-nitroso-1'-demethylnicotine **N169**
N-nitrosodibutylamine **N146**
N-nitrosodi-*sec*-butylamine **N147**
N-nitrosodiethanolamine **N148**
N-nitrosodiethylamine **N149**
 1-nitroso-5,6-dihydrouracil **N150**
N-nitrosodiisopropanolamine **N151**
N-nitrosodiisopropylamine **N152**
N-nitrosodimethylamine **D444**
 4-nitroso-*N,N*-dimethylaniline **D445**
p-nitrosodimethylaniline **D445**
 nitroso-2,6-dimethylmorpholine **N153**
N-nitroso-2,6-dimethylmorpholine **N153**
 4-nitrosodiphenylamine **N154**
N-nitrosodiphenylamine **N155**
p-nitrosodiphenylamine **N154**
N-nitrosodipropylamine **N156**
 nitrosoethanecarbamonitrile **E157**
N-nitroso-*N*-ethylaniline **N157**
N-nitroso-*N*-ethylphenylamine **N157**
 1-nitroso-1-ethylurea **N158**
N-nitroso-*N*-ethylurea **N158**

N-nitrosoheptamethyleneimine **N159**
 nitroso-2-hydroxyethylurea **H111**
 2,2'-(nitrosoimino)bisethanol **N148**
 1,1'-nitrosoiminobis(2-propanol) **N151**
 nitrosoiminodiethanol **N148**
N-nitroso-2-isopropoxyphenyl methylcarbamate **N173**
 nitrosomethylaniline **N160**
N-nitroso-*N*-methylaniline **N160**
N-nitroso-*N*-methylcarbamide **N163**
N-(*N*-nitroso-*N*-methylcarbamoyl)-*L*-ornithine **M268**
N-nitroso-*N*-methylethylamine **N161**
N-nitrosomethylglycine **N175**
N-nitroso-*N*-methyl-*N'*-nitroguanidine **M265**
N-nitrosomethylphenylamine **N160**
N-nitroso-*N*-(1-methylpropyl)-2-butanamine **N147**
 nitrosomethylundecylamine **N162**
N-nitroso-*N*-methylundecylamine **N162**
 1-nitroso-1-methylurea **N163**
N-nitroso-*N*-methylurea **N163**
N-nitroso-*N*-methylurethane **N164**
N-nitroso-*N*-methylvinylamine **N165**
 4-nitrosomorpholine **N166**
N-nitrosomorpholine **N166**
 1-nitroso-2-naphthalenol **N167**
 2-nitroso-1-naphthalenol **N168**
 1-nitroso-2-naphthol **N167**
 2-nitroso-1-naphthol **N168**
 α -nitroso- β -naphthol **N167**
N-nitrososornicotine **N169**
N-nitroso-*N*-pentylurea **A203**
 4-nitrosophenol **N170**
p-nitrosophenol **N170**
 4-nitroso-*N*-phenylaniline **N154**
 4-nitroso-*N*-phenylbenzenamine **N154**
N-nitroso-*N*-phenylbenzenamine **N155**
N-nitroso-*N*-(2-phenylethyl)methylamine **N171**
N-nitrosophenylhydroxylamine, ammonium salt **C476**
 nitrosopiperidine **N172**
 1-nitrosopiperidine **N172**
N-nitrosopiperidine **N172**
 nitrosopropoxur **N173**
N-nitrosopropoxur **N173**
N-nitroso-*N*-propyl-1-propanamine **N156**
 1-nitroso-2-(3-pyridyl)pyrrolidine **N169**
 1-nitrosopyrrolidine **N174**
N-nitrosopyrrolidine **N174**
 3-(1-nitroso-2-pyrrolidinyl)pyridine **N169**
N-nitrososarcosine **N175**
N-nitroso-2,2,4-trimethyl-1,2-dihydroquinoline, polymers **N176**
 1-nitroso-2,2,4-trimethyl-1(2*H*)-quinoline, polymers **N176**
 Nitrosprint **C36**
 nitrosyl chloride **N177**
 4-nitro-2,3,5,6-tetrachloroanisole **T53**
 nitrothale-isopropyl **N178**
 nitrothal-isopropyl **N178**
 Nitrothiamidazole **N62**

Nitrothiazol **N62**
N-(5-nitro-2-thiazolyl)acetamide **A31**
 5-nitro-2-thiazolylamine **A141**
 1-(5-nitro-2-thiazolyl)-2-imidazolidinone **N62**
 2-nitrotoluene **N179**
 3-nitrotoluene **N180**
 4-nitrotoluene **N181**
m-nitrotoluene **N180**
o-nitrotoluene **N179**
p-nitrotoluene **N181**
 2-nitro-*p*-toluidine **M261**
 3-nitro-*p*-toluidine **M262**
 4-nitro-2-toluidine **M259**
 5-nitro-4-toluidine **M262**
 5-nitro-*o*-toluidine **M260**
m-nitro-*p*-toluidine **M262**
 4-nitrotoluol **N181**
 nitrotriazole **N182**
 3-nitro-1,2,4-triazole **N182**
 3-nitro-1*H*-1,2,4-triazole **N182**
 3-nitro-*s*-triazole **N182**
 nitrotribromomethane **T206**
 nitrotrichloromethane **C259**
 1-nitro-2-trifluoromethylbenzene **N93**
 1-nitro-4-trifluoromethylbenzene **N95**
 2-nitro- α,α,α -trifluorotoluene **N93**
 3-nitro- α,α,α -trifluorotoluene **N94**
 4-nitro- α,α,α -trifluorotoluene **N95**
m-nitrotrifluorotoluene **N94**
 3-nitro-*N*¹,*N*¹,*N*⁴-tris(2-hydroxyethyl)-*p*-phenylenediamine
 H8
 nitrous acid, ethyl ester **E156**
 nitrous acid, potassium salt **P258**
 nitrous acid, sodium salt **S81**
 nitrous anhydride **D479**
 nitrous ether **E156**
 nitrous oxide **N183**
 nitrovin **N184**
 Nitrox **P14**
 nitroxanthic acid **P187**
 2-nitro-1,3-xylene **N185**
 2-nitro-*m*-xylene **N185**
 3-nitro-*o*-xylene **N186**
 4-nitro-1,3-xylene **N187**
 4-nitro-*m*-xylene **N187**
 4-nitro-*o*-xylene **N188**
 Nivemycin **N34**
 Nivral **T128**
 NK 049 **M145**
 NK 711 **L35**
 NK Ester A-NPG **N41**
 NMEA **N161**
 NMO **M39**
 NMOR **N166**
 NMU **N163**
 NMUT **N164**
 NNF-136 **F92**
 NNK **N189**
 NNN **N169**
 Nobese **N203**
 Nobilen **T145**
 Noctec Capsules **C108**
 Noctosom **F84**
 NO-DHU **N150**
 Noeceler S **S64**
 Nolvadex **T5**
trans-nonachlor **N190**
trans-nonachlordane **N190**
 nonadecanenitrile **N191**
 1,1,2,2,3,3,4,4,4-nonafluoro-*N,N*-bis(nonafluorobutyl)-1-
 butanamine **P55**
 1-nonaldehyde **N192**
 nonanal **N192**
 1-nonanal **N192**
 nonane **N193**
n-nonane **N193**
 nonanenitrile **O21**
 1-nonanethiol **N194**
 nonanoic aldehyde **N192**
 nonan-1-ol **N195**
 1-nonanol **N195**
 Nonion LP 20R **S103**
 Nonox D **P124**
 nonoxynol **N196**
n-nonyl alcohol **N195**
sec-nonyl alcohol **D418**
 nonyl aldehyde **N192**
 nonylcarbinol **D42**
 nonyl hydride **N193**
 nonyl mercaptan **N194**
 nonyl methyl ketone **U6**
 4-nonylphenol **N197**
n-nonylphenol **N198**
p-nonylphenol **N197**
 nonylphenol (mixed isomers) **N198**
p-nonylphenol polyethylene glycol ether **N196**
 nonyltrichlorosilane **N199**
 1-nonyne **N200**
 nopinene **P198**
 NO-PIP **N172**
 Nopocide N-40-D **C286**
 Noprapiophenone **D315**
 NO-propoxur **N173**
 NO-PYR **N174**
 Norantipyrene **P121**
 norbormide **N201**
 norbornadiene **N202**
 2,5-norbornadiene **N202**
 Noreosan **H76**
 norephedrine hydrochloride **N203**
d,l-norephedrine hydrochloride **N203**
 norethindrone **N204**
 norethisterone **N204**
 19-norethisterone **N204**

norethisterone acetate mixture with ethinylestradiol **N207**
 norethynodrel **N205**
 19-nor-17 α -ethynyl-17 β -hydroxy-4-androsten-3-one **N204**
 19-nor-17 α -ethynyltestosterone **N204**
 norflurazon **N206**
 Norgesic **G38**
 Norglycin **T170**
 Norharman **C71**
 Norharmane **C71**
 Noridyl **T203**
 Norinyl **N204**
 Norlestrin **N207**
 Norleucamine **P47**
 normal lead acetate **L12**
 normal lead stearate **L20**
 Norolen **N205**
 Norphenazone **P121**
 (-)-norpinene **P199**
 Norplant **L38**
 (17 α)-19-norpregna-1,3,5(10)-trien-20-yne-3,17-diol **E66**
 19-norpregna-1,3,5(10)-trien-20-yn-17-ol, 3-methoxy-, (17 α)-
M92
 (17 α)-19-norpregna-1,3,5(10)-trien-20-yn-17-ol, mixture
 with (17 α)-3-methoxy-19-norpregna-1,3,5(10)-trien-20-
 yn-17-ol **E28**
 (3 β ,17 α)-19-norpregn-4-en-20-yne-3,17-diol diacetate
E182
 19-norpregn-4-en-20-yne-3,17-diol, diacetate, (3 β ,17 α)-,
 mixed with (17 α)-3-methoxy-19-norpregna-1,3,5(10)-
 trien-20-yn-17-ol **O41**
 19-nor-17 α -pregn-4-en-20-yn-17-ol **L67**
 19-norpregn-4-en-20-yn-17-ol, (17 α)- **L67**
 Norquen' **M92**
 norspermidine **N208**
 Nortron **E72**
 Norvan **F7**
 No Scald **D540**
 Nosemack **T133**
 Nova **M360**
 Novecyl **S5**
 Novodigal **D339**
 Novon **T261**
 Novophone **S146**
 Novox **B271**
 Noxal **D565**
 Noxfish **R18**
 Noxyron **G22**
 1-NP **N138**
 2-NP **N139**
 2-NP **N133**
 NP 48 **A71**
 NPG **E116**
 NPIP **N172**
 2-NPPD **N133**
 NPYR **N174**
 NS130 **N12**
 NS160 **N12**
 NSC-104801 **C547**
 NSC-150014 **H89**
 NSC-26805 **E146**
 NSC-339 **D496**
 NSC-39069 **T195**
 NSC-49842 **V21**
 NSC-66847 **T99**
 NSC-67574 **V25**
 NSC-759 **B53**
 NSC-8722 **A45**
 NSC 63878 **C546**
 NSC-52695 cyclophosphamide cyclohexylamine salt **C548**
 N-Serve **N66**
 N-Serve 24E **N66**
 NTA sodium hydrate **T358**
 NTN 19701 **P19**
 NTN 801 **M41**
 nuarimol **N209**
 nudrin **M126**
 Nu-Flow M **M360**
 Nuocide **C286**
 Nustar **F90**
 Nuvacron **M343**
 Nuvagrain **C314**
 Nuvan **B187**
 Nuvanol N **I50**
 Nydrazin **I109**
 Nysfungin **N210**
 Nystan **N210**
 nystatin **N210**
 Nytek **O50**
 OAP **H52**
 Obeline picrate **A182**
 Obesitex **D315**
 OCBM **C175**
 O-[*p*-[*p*-chlorophenyl]azo]phenyl]-*O*,*O*-dimethyl
 phosphorothioate **A273**
 ochratoxin A **O1**
 (-)-ochratoxin A **O1**
 octacarbonyl dicobalt **C371**
 Octachlor **C118**
 octachlorocamphene **C48**
 octachlorodipropyl ether **B136**
 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-4,7-
 methano-1*H*-indene **C118**
 1,3,4,5,6,7,8,8-octachloro-1,3,3a,4,7,7a-hexahydro-4,7-
 methanoisobenzofuran **I82**
 octachloro-4,7-methanotetrahydroindane **C118**
 octachloronaphthalene **O2**
 1,2,4,5,6,7,8,8-octachloro-3a,4,7,7a-tetrahydromethanoindan
C118
 1,3,4,5,6,7,8,8-octachloro-3a,4,7,7a-tetrahydro-4,7-
 methanoisobenzofuran **I82**
 9,12-octadecadienoic acid, (Z,Z)- **L49**
 1-octadecanamine **S111**
 1-octadecanethiol **O3**
 octadecanoic acid **S112**

octadecanoic acid, cadmium salt **C12**
 octadecanoic acid, lead salt **L20**
 octadecanoic acid, zinc salt **Z16**
 octadecan-1-ol **S113**
 1-octadecanol **S113**
 (Z)-9-octadecen-1-amine **O28**
 cis- Δ^9 -octadecenoic acid **O31**
 (E)-9-octadecenoic acid **O30**
 trans- Δ^9 -octadecenoic acid **O30**
 (Z)-9-octadecenoic acid **O31**
 9-octadecenoic acid, (Z)-, mercury salt **M80**
 9-octadecenoic acid, methyl ester, (Z)- **M270**
 9-octadecenoic acid, oxiranylmethyl ester **G34**
 cis-9-octadecenylamine **O28**
 octadecyl alcohol **S113**
 octadecylamine **S111**
 octadecyl mercaptan **O3**
 octadecyltrichlorosilane **O4**
 octafluoro-2-butene **O5**
 octafluorobut-2-ene **O5**
 octafluoro-sec-butene **O6**
 1,1,1,2,3,4,4,4-octafluoro-2-butene **O5**
 octafluoroisobutene **O6**
 octafluoroisobutylene **O6**
 octafluoropropane **O7**
 octahydro-4,8a-dimethyl-4a(2H)-naphthalenol **G11**
 octahydro-1-nitrosoazocine **N159**
 octamethyldiphosphoramidate **S9**
 octamethylpyrophosphoramidate **S9**
 octamethylpyrophosphoric tetramide **S9**
 octanal **O8**
 octanaldehyde **O8**
 octane **O9**
 n-octane **O9**
 1,8-octanedicarboxylic acid **S11**
 1-octanethiol **O10**
 tert-octanethiol **O11**
 octanoic acid **O12**
 n-octanoic acid **O12**
 octanoic acid, 2-propenyl ester **A89**
 octanoic acid triglyceride **T224**
 1-octanol **O13**
 2-octanol **O14**
 3-octanol **O15**
 2-octanone **O16**
 3-octanone **E91**
 4-octanone **O17**
 octanylic acid **O12**
 1-octen-3-ol **O18**
 octhelinone **O19**
 octic acid **O12**
 octilin **O13**
 Octopol SDE-25 **D575**
 Octowet 40 **D583**
 octoxanil **O20**
 octoxynol **O20**
 sec-octyl acrylate **E131**
 octyl adipate **D513**
 octyl alcohol **O13**
 2-octyl alcohol **O14**
 sec-octyl alcohol **O14**
 n-octyl aldehyde **O8**
 octyl carbinol **N195**
 octyl cyanide **O21**
 octyl decyl phthalate **O22**
 n-octyl n-decyl phthalate **O22**
 octylene epoxide **E39**
 octylene glycol **E126**
 octyl hydrogen phthalate **M346**
 octylic acid **O12**
 2-n-octyl-4-isothiazolin-3-one **O19**
 2-octyl-3(2H)-isothiazolone **O19**
 n-octyl mercaptan **O10**
 tert-octyl mercaptan **O11**
 4-octyl-N-(4-octylphenyl)benzeneamine **D516**
 tert-octylphenol **O23**
 1-octyl thiol **O10**
 octyltin chloride **O24**
 octyltrichlorostannane **O24**
 Ocuser Pilo **P189**
 oenan thanldehyde **H19**
 oenanthic acid **H22**
 oenanthol **H19**
 oestradiol **E50**
 17 β -oestradiol **E50**
 oestriol **O25**
 Oestromenin **S116**
 oestrone theelin **E53**
 Oftanol **I103**
 ofurace **O26**
 Ohio 347 **E27**
 Oibrom **N3**
 oil mist, mineral **M333**
 Oil of Niobe **M161**
 oil of turpentine **T374**
 oil of vitriol **S152**
 Oil Orange **C426**
 Oil Orange R **C420**
 Oil Orange SS **O27**
 Oil Red **C422**
 Oil Red O **C420**
 Oil Scarlet BL **C420**
 oils, rosin **R17**
 Oil Yellow N **M320**
 Oil Yellow SIS **C427**
 oleamine **O28**
 oleandomycin **O29**
 oleate of mercury **M80**
 olefiant gas **E113**
 (E)-oleic acid **O30**
 (Z)-oleic acid **O31**
 oleic acid, 2,3-epoxypropyl ester **G34**
 oleic acid, glycidyl ester **G34**
 cis-oleic acid, methyl ester **M270**

oleinamine **O28**
 oleum **S153**
 oleylamine **O28**
 Olothorb **P230**
 omadine zinc **Z15**
 Omaflora **H91**
 Omal **T259**
 omethoate **O32**
 Omite **P300**
 OMS 1211 **I50**
 OMS 1809 **P84**
 OMS 1810 **P84**
 OMS 2005 **M102**
 OMS 712 **D460**
 ONB **N98**
 Oncol **B30**
 Oncostatin K **A46**
 Onecide **F38**
 Oneovin **V25**
 Oniachlor 90 **T250**
 onion oil **A92**
 ONT **N179**
 onyx **Q1**
 Onyxide 200 **H51**
 opal **S29**
 Ophthalgan **G25**
 Ophthalmadine **I48**
 Opilon **T155**
 Ophthalamine **R7**
 Op-thal-zin **Z17**
 Optimax **T369**
 Oraldene **H75**
 Oraline **T171**
 Orange G.C. Base **C155**
 Oratrast **B24**
 Orbisan **T120**
 Oranon **M312**
 orciprenaline **O33**
 Ordoval **H80**
 Ordram **M337**
 Orestol **S117**
 Oretic **H94**
 Orfiril **S100**
 orgametril **L67**
 Organex **C20**
 Orisul **S139**
 orlest **N207**
 Ornaline **V23**
 Ornamite **P300**
 Orobronze **C413**
 Oropur **O34**
 otrotic acid **O34**
 orphenadrine **O35**
 orthamine **P102**
 orthanilic acid **A211**
 Orthene **A5**
 orthoarsenic acid **A241**

Orthocid **C59**
 Orthocide-406 **C59**
 Ortho Difolatan **C58**
 orthoformic acid, ethyl ester **T286**
 orthoformic acid, trimethyl ester **T313**
 orthohydrogen **H96**
 Orthonal **M119**
 Orthonovum **N204**
 Ortho Phosphate Defoliant **T209**
 orthophosphoric acid **P156**
 Orthorix **C42**
 Ortho Spotless **D464**
 orthotoluic acid **T182**
 Orthotox **M111**
 Ortus **F21**
 Orudis **K10**
 Oruvail **K10**
 oryzalin **O36**
 Osadan **F7**
 Osbac **F12**
 Osbon AC **P51**
 Oscaf **Z10**
 osmic acid **O39**
 Osmitol **M28**
 osmium **O37**
 osmium chloride **O38**
 osmium oxide (OsO₄), (T-4)- **O39**
 osmium tetrachloride **O38**
 osmium tetroxide **O39**
 Osmoglyn **G25**
 Ospalivina **M352**
 osyritrin **R22**
 Ottasept Extra **C306**
 ouabain **O40**
 Ovaban **M44**
 Ovatox **D510**
 Overdyn **C68**
 Overtop **I7**
 Ovestin **O25**
 Ovex **C127**
 ovulen **O41**
 10H-9-oxaanthracene **X1**
 oxabetrinil **O42**
 7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylic acid **E22**
 7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylic acid, disodium salt **E23**
 6-oxabicyclo[3.1.0]hexane **O43**
 oxacyclobutane **T309**
 oxacyclopentadiene **F123**
 oxacyclopentane **T72**
 oxacyclopropane **E120**
 oxadiazon **O44**
 2-oxa-3,3-dimethylbutane **M181**
 oxadixyl **O45**
 Oxafuradene **N58**
 3-oxaheptane **B257**
 oxal **G39**

oxaldehyde **G39**
 oxalgon **P218**
 oxalic acid **O46**
 oxalic acid, copper(II) salt (1:1) **C439**
 Oxalid **O63**
 oxalonitrile **C482**
 oxalyl cyanide **C482**
 oxamimidic acid, (N',N')-dimethyl-N-[methylcarbamoyl]-oxy]-1-thio-, methyl ester **O47**
 oxammonium **H112**
 oxamyl **O47**
 5-oxanonane **D145**
 oxanthrene **D106**
 3-oxapentane **D304**
 3-oxa-1-pentene **E181**
 2-oxapropane **D413**
 1,2-oxathiane-2,2-dioxide **B210**
 1,4-oxathiin-3-carboxamide, 5,6-dihydro-2-methyl-N-phenyl **C84**
 1,4-oxathiin-3-carboxanilide, 5,6-dihydro-2-methyl- **C84**
 1,2-oxathiolane 2,2-dioxide **P293**
 Oxatin **C84**
 oxazepam **O48**
 oxazolidinone hydrochloride **O49**
 oxetane **T309**
 2-oxetanone **P308**
 2-oxetanone, 4-methyl- **B287**
 Oxidation base 25 **A140**
 2-oximinobutane **M221**
 1-oxindene **B61**
 oxine **H119**
 oxine-copper **O50**
 oxine sulfate **H120**
 oxirane **E120**
 oxiranecarboxaldehyde **G27**
 oxiranemethanol **G28**
 oxirane polymer **P225**
 oxiranylmethanol **G28**
 N-(oxiranylmethyl)-N-phenyl-oxiranemethanamine **D336**
 oxiranylmethyl 2-propenoate **G29**
 3-oxiranyl-7-oxabicyclo[4.1.0]heptane **V32**
 Oxitol **E76**
 oxitol acetate **E79**
 2-oxobornane **C51**
 3-oxo-butanoic acid butyl ester **B236**
 δ -oxo- α -butylene **M318**
 3-oxo-L-gulofuranolactone sodium enolate **S46**
 2-oxohexamethylenimine **C55**
 oxohydrindene **I20**
 oxole **F123**
 oxomethane **F100**
 2-oxo-6-methylhept-5-ene **M232**
 4-oxo-pentanoic acid **L40**
 2-oxopropanoic acid **P368**
 4-oxopterine **P345**
 oxo[sulfato(2-)-O]vanadium **V16**
 1-oxo-1,2,3,4-tetrahydronaphthalene **T83**
 1-oxotetralin **T83**
 oxotremorin **O51**
 oxotremorine **O51**
 2-oxo-1,7,7-trimethylbicyclo[2.2.1]heptane **C50**
 4-oxovaleric acid **L40**
 22-oxovinaleukoblastine sulfate **V25**
 22-oxovincal leukoblastine **V24**
 9-oxoxanthene **X3**
 oxprenolol **O52**
 Oxsoralen-Ultra **M129**
 4,4'-oxybis(aniline) **O58**
 4,4'-oxybisbenzenamine **O58**
 1,1'-oxybisbenzene **D544**
 4,4'-oxybis(benzenediamine) **O58**
 4,4'-oxybis(benzenesulfonyl hydrazide) **O53**
 1,1'-oxybis(4-bromobenzene) **B115**
 1,1'-oxybis(butane) **D145**
 4,4'-oxybis(2-chloroaniline) **O54**
 4,4'-oxybis(2-chlorobenzenamine) **O54**
 1,1'-oxybis(2-chloro)ethane **B120**
 oxybis[chloromethane] **B123**
 2,2'-oxybis(1-chloropropane) **D26**
 1,1'-oxybis[ethane] **D304**
 1,1'-oxybisethene **D581**
 1,1'-oxybis(2-ethoxyethane) **E80**
 2,2'-(oxybis(ethyleneoxy))diethanol **T64**
 oxybismethane **D413**
 1,1'-oxybis[2-methoxyethane] **D338**
 2,2'-[oxybis(methylene)]bisoxirane **D337**
 1,1'-oxybis[2,3,4,5,6-pentabromobenzene] **P24**
 1,1'-oxybispentane **P48**
 10,10'-oxybisphenoxarsine **O55**
 10,10'-oxybis-10H-phenoxarsine **O55**
 1,1'-oxybispropane **D557**
 2,2'-oxybispropane **D359**
 3,3'-oxybis-1-propene **D71**
 1,1'-oxybis[2,3,3,3-tetrachloropropane] **B136**
 oxybis(trimethylsilane) **H53**
 oxybutyric aldehyde **A63**
 oxycarbon sulfide **C81**
 oxycarbophos **M10**
 oxycarboxin **O56**
 oxychinolin **H119**
 oxydemeton-methyl **O57**
 4,4'-oxydianiline **O58**
 Oxydiazol **M120**
 4,4'-oxydibenzene sulfonyl hydrazide **O53**
 2,2'-oxydiethanol **D301**
 2,2'-oxydiethyl diacrylate **D302**
 oxydiethylene acrylate **D302**
 oxydiethylene diacrylate **D302**
 oxydifluoride **O61**
 10,10'-oxydiphenoxarsine **O55**
 1,1'-oxydi-2-propanol **D555**
 oxydisulfoton **D567**
 oxyfluorfen **O59**
 oxygen **O60**

oxygen difluoride **O61**
 oxygen fluoride (OF₂) **O61**
 Oxy-Gro-G **C39**
 Oxy-Gro-T **C39**
 oxymethenolone **O62**
 oxymetholone **O62**
 oxymethylene **F100**
 Oxymycin **O64**
 oxy-NH₂ **M39**
 oxyphenbutazone **O63**
 oxypsoralen **M129**
 Oxypure **H103**
 oxyquinoline **H119**
 oxyquinoline sulfate **H120**
 oxysulfatovanadium **V16**
 Oxytetracid **O64**
 oxytetracycline **O64**
 oxythioquinox **Q11**
 oxytremorine **O51**
 ozone **O65**
 P128 **L31**
 P37 **L31**
 PABA **A117**
 PAC **C131**
 6β,7α,9α,11α-pachycarpine **S105**
 paclobutrazol **P1**
 Padan **C92**
 PAG DLTDP **D365**
 Palatase **L51**
 Palatinol DIDP **D355**
 Palatinol DOA **D514**
 Palatinol DOP **D519**
 Palatinol IC **D354**
 Palatinol M **D450**
 palladium chloride **P2**
 palladium(II) chloride **P2**
 palladium dichloride **P2**
 palladous chloride **P2**
 palmityl alcohol **C102**
 Palohex **I38**
 L-PAM **M49**
 Pamanrin **F21**
 Pamolyn **L49**
 Panacet 800 **T224**
 Panacide **D235**
 Panatac **C357**
 Panazone **N184**
 Pancil **O19**
 Pandrinol **M251**
 Panfuran-S **D350**
 Pannox 18 **N196**
 Panocon **F15**
 Panogen **M137**
 Panogen PX **M251**
 Panoram **F10**
 Pansoil **E185**
 Pantherine **M356**
 Pantomicina **E47**
 Panwarfin **W3**
 papain **P3**
 papainase **P3**
 papaverin **P4**
 papaverine **P4**
 papaverine chlorhydrate **P5**
 papaverine hydrochloride **P5**
 Papavorsan **P5**
 Papayotin **P3**
 Paperon **P5**
 paraacetaldehyde **P9**
 paracetaldehyde **P9**
 paracetamol **P6**
 Paracide **D190**
 Paracodin **D344**
 Paracortol **P269**
 paradormalene **M117**
 paraffin oil **M333**
 paraffin wax **P7**
 paraffin waxes and hydrocarbon waxes, chlorinated **C133**
 paraffin waxes and hydrocarbon waxes, chlorinated **C134**
 Paraform **P8**
 paraformaldehyde **P8**
 parahydrogen **H96**
 Parakakes **P193**
 Paral **P9**
 paraldehyde **P9**
 paraminol **A117**
 paraminopropiophenone **A149**
 Paramouth **D190**
 paranaphthalene **A218**
 paranol **A144**
 paraoxon **P10**
 Paraphos **P13**
 paraquat **P11**
 paraquat dication **P11**
 paraquat ion **P11**
 pararosanine chloride **C402**
 parascorbic acid **P12**
 parathion **P13**
 parathion-methyl **P14**
 paraxenol **P127**
 pardopa **L37**
 Pargonyl **N38**
 Paridol Butyl **B269**
 Paridol Ethyl **E158**
 Paridol Methyl **M272**
 Paridol Propyl **P336**
 Paris Green **P15**
 Parrot **C99**
 parsley apiole **A230**
 parsley camphor **A230**
 pasco **Z2**
 passiflorin **H6**
 Patent Blue VF **C386**
 Patonex **M322**

Patoran **M322**
 Patrol **F19**
 Patrol **M111**
 patulin **P16**
 Paxilon **M120**
 Pay-Off **F43**
 Payzone **N184**
 PBB **P219**
 PBO-9 **P204**
 PCA **C131**
 PCB **A233**
 PCB 1242 **A236**
 PCB 1254 **A238**
 PCB 1260 **A239**
 PCHO **P9**
 PCMC **C183**
 PCNB **Q12**
 PCP **P30**
 PCPA **C452**
 PCT **P220**
 PDCB **D190**
 PDU **F27**
 PEA **P67**
 pear oil **I80**
 PEBC **P17**
 pebulate **P17**
 Pediaflor **S66**
 PEG **P225**
 PEG *p*-nonylphenyl ether **N196**
 PEHA **P38**
 Pelagol CD **P105**
 Pelagon D **P103**
 pelargonaldehyde **N192**
 pelargonic alcohol **N195**
 pelargonic aldehyde **N192**
 pelargonitrile **O21**
 Pelt **T137**
 Pelt 44 **T138**
 Pelton BR II **P128**
 penchlorol **P30**
 penconazole **P18**
 pencycuron **P19**
 pendimethalin **P20**
 Penetek **P35**
 penferate **P215**
 penicidin **P16**
 penicillic acid **P21**
 penicillin **P22**
 Penick **R4**
 Pennad 150 **D289**
 Pennae ZT **Z10**
 Penncap **P14**
 Penncapthrin **R4**
 Pennezone E 0686 **D318**
 Pennstyl **C535**
 penoxalin **P20**
 1,4,7,10,13-pentaazatridecane **T65**
 pentaborane **P23**
 pentaborane(9) **P23**
 pentaboron nonahydride **P23**
 pentabromophenyl ether **P24**
 Pentac **D277**
 pentacarbonyliron **I75**
 pentachloroacetone **P25**
 2,3,4,5,6-pentachloroanisole **P26**
 pentachloroantimony **A223**
 pentachlorobenzene **P27**
 pentachloroethane **P28**
 pentachloromethoxybenzene **P26**
 pentachloronaphthalene **P29**
 pentachloronitrobenzene **Q12**
 pentachlorophenate sodium **S82**
 pentachlorophenol **P30**
 pentachlorophenol, sodium salt **S82**
 pentachlorophenoxy sodium **S82**
 pentachlorophenyl chloride **H33**
 pentachlorophenyl methyl ether **P26**
 pentachlorophosphorane **P160**
 1,1,2,2,3-pentachloropropane **P31**
 1,1,2,3,3-pentachloropropane **P32**
 pentachloro-2-propanone **P25**
 pentachloropropan-2-one **P25**
 1,1,1,3,3-pentachloropropanone **P25**
 1,1,1,3,3-pentachloro-2-propanone **P25**
 $\alpha,\alpha,\alpha,2,4$ -pentachlorotoluene **D197**
 pentadecafluorooctanoic acid, ammonium salt **A180**
 1-pentadecanamine **P33**
 pentadecylamine **P33**
 1-pentadecylamine **P33**
n-pentadecylamine **P33**
 1,3-pentadiene **P34**
 pentaerythritol **P35**
 pentaerythritol dibromide **D134**
 pentaerythritol tetraacrylate **P36**
 pentaerythritol tetrabromide **P37**
 pentaerythrityl bromide **P37**
 pentaerythrityl tetrabromide **P37**
 pentaethylenhexamine **P38**
 pentafluorochloroethane **C234**
 pentafluorophosphorane **P161**
 Pentagin **P42**
 3,3',4',5,7-pentahydroxyflavone **Q2**
 γ -pentalactone **V3**
 pentalin **P28**
 pentamethylene **C522**
 pentamethylene bromide **D136**
 pentamethylene chloride **D234**
 pentamethylene dibromide **D136**
 pentamethyleneimine **P201**
 pentanal **V1**
 1-pentanamine **P47**
 Pentanate **T261**
 pentane **P39**
n-pentane **P39**

tert-pentane **N39**
 1,5-pentanedial **G21**
 pentane-2,3-dione **P40**
 2,3-pentanedione **P40**
 2,4-pentanedione **A22**
 1-pentanethiol **A201**
 pentanoic acid **V2**
 1-pentanol **P41**
tert-pentanol **M173**
 1-pentanol acetate **A195**
 2-pentanol acetate **P46**
 4-pentanoline **V3**
 pentan-2-one **M292**
 pentan-3-one **D307**
 2-pentanone **M292**
 3-pentanone **D307**
 Pentaphen **A205**
 Pentasol **P41**
 pentazocine **P42**
 Pentek **P35**
 1-pentene **P43**
 3-penten-2-one **P44**
 pentiformic acid **H64**
p-pentine **C528**
 pentobarbitone **P45**
 pentobarbituric acid **P45**
 pentole **C528**
 Pentoxane **M140**
 Pentrexyl **A194**
 pentyl acetate **A195**
 1-pentyl acetate **A195**
 2-pentyl acetate **P46**
tert-pentyl acetate **A196**
 pentyl alcohol **P41**
tert-pentyl alcohol **M173**
 pentylamine **P47**
 1-pentylamine **P47**
n-pentylamine **P47**
 pentyl butyrate **A197**
 pentylcarbinol **H65**
 pentyl chloride **A198**
 6-*n*-pentyl-*m*-cresol **A199**
 pent-2-yl ethanoate **P46**
 pentyl ether **P48**
 pentylformic acid **H64**
 pentyl ketone **U7**
 pentylmercaptan **A201**
n-pentyl methyl ketone **H23**
n-pentyl nitrate **A202**
N-pentyl-*N*-nitrosoourea **A203**
N-pentyl-1-pentanamine **D533**
 4-*tert*-pentylphenol **A205**
p-*tert*-pentylphenol **A205**
n-pentyl propanoate **P49**
 pentyl propionate **P49**
n-pentyl propionate **P49**
 pentylsilicon trichloride **A206**
 pentyltrichlorosilane **A206**
 Pentymalum **A204**
 PEO **P225**
 PEP **P223**
 Pepna **O2**
 peppermint camphor **M54**
 Pepsin inhibitor S 735A **P50**
 pepstatin A **P50**
 peracetic acid **P51**
 perchloric acid **P52**
 perchloric acid, barium salt **B15**
 perchloric acid, lead salt **L26**
 perchloric acid, magnesium salt **M7**
 perchloric acid, potassium salt **P259**
 perchloric acid, sodium salt **S83**
 perchlorobenzene **H33**
 perchlorobutadiene **H34**
 perchlorocyclopentadiene **H35**
 perchloroethylene **T51**
 perchloromethane **C78**
 perchloromethyl mercaptan **T252**
 perchloronaphthalene **O2**
 perchloryl fluoride **P53**
 Perclene **T51**
 Percosolve **T51**
 Percumyl D **D264**
 perfluidone **P54**
 perfluoroacetic acid **T290**
 perfluoroacetic anhydride **T291**
 perfluoroacetone **H45**
 perfluorobut-2-ene **O5**
 perfluoro-2-butene **O5**
 perfluoroethane **H46**
 perfluoroethene **T70**
 perfluoroethylene **T70**
 perfluoroisobutylene **O6**
 perfluoromethane **C79**
 perfluoropropane **O7**
 perfluoro-2-propanone **H45**
 perfluoropropene **H48**
 perfluoropropylene **H48**
 perfluorotributylamine **P55**
 perhydroazepine **H56**
cis-perhydronaphthalene **D38**
trans-perhydronaphthalene **D39**
 perhydropyridine **P201**
 periethylenenaphthalene **A3**
 perilene **P57**
 periodin **P259**
 Perizin **C446**
 Perkacit DPG **D545**
 Perkacit ETU **E122**
 Perkacit TDEC **E174**
 Perkacit TETD **D565**
 Perkadox BC **D264**
 Perkadox 14/40C **D154**
 Perlex Paste 500 **L27**

permanganate of potash **P260**
 permanganic acid, barium salt **B16**
 permanganic acid (HMnO₄), calcium salt **C38**
 Permanone **P56**
 permethrin **P56**
 perméthrine **P56**
 Permutine **T134**
 Perone **H103**
 Peropal **A270**
 peroxide, 1-hydroperoxycyclohexyl 1-hydroxycyclohexyl **C510**
 Peroximon F100 **D154**
 Peroximon F40 **D154**
 peroxyacetic acid **P51**
 peroxyacetic acid **P51**
 peroxyacetic acid, *tert*-butyl ester **B270**
 peroxybenzoic acid, *tert*-butyl ester **B271**
 peroxydicarbonic acid, bis(1-methylethyl) ester **D360**
 peroxydicarbonic acid, bis(2-methylpropyl) ester **D153**
 peroxydicarbonic acid, dibutyl ester **D152**
 peroxydicarbonic acid, di-*sec*-butyl ester **D153**
 peroxydicarbonic acid, diisopropyl ester **D360**
 peroxydisulfuric acid, dipotassium salt **P261**
 peroxyisobutyric acid, *tert*-butyl ester **B272**
 peroxyipivalic acid, *tert*-butyl ester **B273**
 Persadox **B83**
 Persulon **F81**
 perylene **P57**
 Pestan **M37**
 petersilienapirole **A230**
 Petrac Eramide **E46**
 petrol **G8**
 petroleum gases, liquefied **L59**
 petroleum naphtha **N5**
 petroleum pitch **A249**
 Petrol Yellow **M320**
 Pezetamid **P348**
 Pfizerquine **C281**
 PGDN **P329**
 Phaltan **F97**
 phemerol chloride **B51**
 phenacetin **P58**
 Phenachlor **T259**
 phenacide **C48**
 phenacyl chloride **C148**
 phenalzine **P65**
 Phenamine Scarlet 3B **C408**
 Phenamine Sky Blue **C405**
 Phenaminosulf **F2**
 phenanthrene **P59**
 1,10-phenanthroline **P60**
 4,5-phenanthroline **P60**
 o-phenanthroline **P60**
 phenazarsine chloride **D541**
 phenazine **P61**
 phenazodine **P63**
 Phenazon **C131**
 phenazopyridine **P62**
 phenazopyridine hydrochloride **P63**
 phencapton **P77**
 Phendal **P89**
 phenelzine dihydrogen sulfate **P64**
 phenelzine sulfate **P64**
 Phenesterin **P65**
 phenesterine **P65**
 phenethanol **P67**
 phenethyl acetate **P66**
 phenethyl alcohol **P67**
 2-phenethyl alcohol **P67**
 α-phenethyl alcohol **P68**
sec-phenethyl alcohol **P68**
 phenethylamine **P69**
 1-phenethylbiguanide **P74**
 phenethylene **S126**
 phenethylene oxide **S127**
 phenethyl isothiocyanate **P70**
 phenethyl mustard oil **P70**
 4-phenetidine **P72**
 o-phenetidine **P71**
 p-phenetidine **P72**
 p-phenetolcarbamide **E81**
 phenetole **P73**
 p-phenetylurea **E81**
 phenformin **P74**
 phenicarbazide **P75**
 phenidone **P76**
 Phenin **P58**
 phenisobromolate **B187**
 phenkapton **P77**
 phenmedipham **P78**
 Phenobarbital **P79**
 phenobarbitone **P79**
 phenodioxin **D106**
 Phenohep **H38**
 phenol **P80**
 Phenolax **P81**
 phenol benzoate **P94**
 phenol, o-*sec*-butyl **B275**
 phenol, *tert*-butyl-4-methoxy-*tert*-butyl-4-hydroxyanisole **B244**
 phenol, 2-chloro-4,5-dimethyl-, methylcarbamate **C62**
 phenol, 2,4-diamino- **D81**
 phenol, 2,4-dichloro-6-nitro- **D233**
 phenol, 4,4'-(1,2-diethyl-1,2-ethenediyl)bis-, dipropanoate, (E)- **S117**
 phenol, 4-[2-(dimethylamino)ethoxy]-2-methyl-5-(1-methylethyl)-, acetate (ester) **T155**
 phenol, 4-(1,1-dimethylethyl)- **B276**
 phenol, (1,1-dimethylethyl)-4-methoxy- **B244**
 phenol, 4-fluoro- **F70**
 phenol, 2-methoxy-4-(2-propenyl)- **E187**
 phenol, 2-(1-methylpropyl) **B275**
 phenol, 2-(1-methylpropyl)-4,6-dinitro- **D510**
 phenolphthalein **P81**

phenol sodium **S85**
 phenol trinitrate **P187**
 phenopyridine **H119**
 phenosafranin **P82**
 phenosafranin **P82**
 phenothiazine **P83**
 10H-phenothiazine **P83**
 10H-phenothiazine, 10-[2-(1-methyl-2-piperidinyl)ethyl]-2-(methylthio)- **T143**
 phenothiazine, 10-[2-(1-methyl-2-piperidyl)ethyl]-2-(methylthio)- **T143**
 Phenothiol **M33**
 phenothrin **P84**
 Phenoverm **P83**
 3H-phenoxazine, actinomycin C deriv. **A45**
 3H-phenoxazine, actinomycin D deriv. **A46**
 phenoxethol **P86**
 phenoxybenzamine chloride **P85**
 phenoxybenzamine hydrochloride **P85**
 phenoxybenzene **D544**
 3-phenoxybenzyl *cis,trans*-chrysanthemate **P84**
 3-phenoxybenzyl(1*RS*,3*RS*;1*RS*, 3*SR*)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate **P56**
 S-(4-phenoxybutyl)dimethylthiocarbamate **F15**
 S-4-phenoxybutyl *N,N*-dimethylthiocarbamate **F15**
 2-phenoxybenzylphenol **P132**
 1-phenoxy-2,3-epoxypropane **G35**
 phenoxyethane **P73**
 2-phenoxyethanol **P86**
 β-phenoxyethyl alcohol **P86**
 (±)-*m*-phenoxyhydratropic acid **F13**
 (phenoxymethyl)oxirane **G35**
 4-phenoxyphenol **P87**
p-phenoxyphenol **P87**
 phenoxypropylene oxide **G35**
 phenoxythrin **P84**
 Phenozin **Z13**
 phenpropanage **F18**
 phentermine **P88**
 phenthoate **P89**
 phenudin **P77**
 phenudine **P77**
N-phenylacetamide **A11**
 6-phenylacetamidopenicillanic acid **B100**
 4-phenylacetanilide **P90**
p-phenylacetanilide **P90**
 phenylacetic acid, allyl ester **A91**
 phenylacetic acid chloride **P91**
 phenylacetonitrile **B97**
 phenylacetyl chloride **P91**
 α-phenylacetyl chloride **P91**
 phenylacrolein **C346**
 β-phenylacrolein **C346**
 phenylalanine **P92**
 3-phenylalanine **P92**
 β-phenylalanine **P92**
 L-phenylalanine **P92**
 DL-phenylalanine, 4-[bis(2-chloroethyl)amino]- **M88**
 phenylalanine mustard **M49**
 DL-phenylalanine mustard **M88**
 phenyl alcohol **P80**
 γ-phenylallyl formate **C348**
 phenylamine **A209**
 4-(phenylamino)aniline **P128**
 4-(phenylamino)butane **B242**
 2-[(phenylamino)carbonyl]benzoic acid **P130**
 [3-[(phenylamino)carbonyl]oxy]phenyl]carbamic acid, ethyl ester **D59**
 1-phenyl-4-amino-5-chloropyridaz-6-one **C131**
 1-phenyl-2-aminopropane **A193**
 2-phenylaniline **A119**
 3-phenylaniline **A120**
m-phenylaniline **A120**
N-phenylaniline **D540**
o-phenylaniline **A119**
p-phenylaniline **A121**
 phenylarsenic acid **P93**
 phenyl arsenous dichloride **P98**
 phenylarsine dichloride **P98**
 phenylarsonic acid **P93**
 4-phenylazoaniline **A114**
p-(phenylazo)aniline **A114**
 4-(phenylazo)-1,3-benzenediamine **D79**
 1-(phenylazo)-2-naphthalenol **C426**
 1-phenylazo-β-naphthol **C426**
 4-(phenylazo)phenol **C425**
 1-[[4-(phenylazo)phenyl]azo]-2-naphthalenol **C422**
 1-(*p*-phenylazophenylazo)-2-naphthol **C422**
 4-phenylazo-*m*-phenylenediamine **D79**
 3-(phenylazo)-2,6-pyridinediamine **P62**
 3-(phenylazo)-2,6-pyridinediamine, monohydrochloride **P63**
 (phenylazo)thioformic acid 2-phenylhydrazide **D576**
N-phenylbenzenamine **D540**
 phenylbenzene **B113**
N-phenyl-1,4-benzenediamine **P128**
 2-phenyl-1,4-benzenediol **P110**
 2-phenyl-1*H*-benzimidazole, **P143**
 phenyl benzoate **P94**
 2-phenyl-4*H*-1-benzopyran-4-one **F36**
 3-phenyl-4*H*-1-benzopyran-4-one **I104**
 phenylbiguanide **P95**
 1-phenylbiguanide **P95**
 2-phenylbiphenyl **T30**
 4-phenylbiphenyl **T31**
N-[3-phenyl-4,5-bis[(trifluoromethyl)imino]-2-thiazolidinylidene]benzenamine **F40**
 phenyl bromide **B161**
 1-phenylbutane **B246**
 phenylbutazone **P96**
 phenyl-*tert*-butylamine **P88**
 phenylcarbamic acid, 1-methylethyl ester **P305**
 phenylcarbimide **P113**
 phenylcarbinol **B89**

phenyl carbonimide **P113**
 phenylcarboxy amide **B42**
 phenyl cellosolve **P86**
 phenylchloramine **C157**
 phenyl chloride **C163**
 phenyl chlorocarbonate **P97**
 phenylchloroform **B79**
 phenyl chloroformate **P97**
 phenyl chloromercury **P118**
 phenyl chloromethyl ketone **C148**
 4-phenyl-2-chlorophenol **C249**
 2-phenylchromone **F36**
 3-phenylchromone **I104**
 phenyl cyanide **B68**
 1-phenyldecane **D44**
 phenyldiazenecarbothioic acid 2-phenylhydrazide **D576**
 2-phenyldiazenecarboxamide **P75**
 phenyldichloroarsine **P98**
 phenyldichlorophosphine **D242**
 phenyl-5,6-dichloro-2-(trifluoromethyl)benzimidazole-1-carboxylate **F5**
 phenyl-5,6-dichloro-2-(trifluoromethyl)-1H-benzimidazole-1-carboxylate **F5**
 1-phenyl-2-diethylamino-1-propanone **D315**
 2-phenyl-4,5-dihydroimidazole **P112**
 3-phenyl-1,1-dimethylurea **F27**
 3-phenyldiphenyl **T29**
 2-phenyl-1,3-dithiane **P99**
 2-phenyl-*m*-dithiane **P99**
 1-phenyldodecane **P100**
 [1,2-phenylenebis(carbonyloxy)]bis[tributylstannane] **T220**
m-phenylenebis(methylamine) **X17**
 1,4-phenylenebis(1-methylethylidene) bis(1,1-dimethylethyl peroxide) **D154**
 2,2'-[1,3-phenylenebis(oxyethylene)]bisoxirane **R6**
m-phenylenediamine **P101**
o-phenylenediamine **P102**
p-phenylenediamine **P103**
p-phenylenediamine, 2,6-dichloro- **D240**
m-phenylenediamine dihydrochloride **P104**
p-phenylenediamine dihydrochloride **P105**
m-phenylenediammonium dichloride **P104**
m-phenylene dichloride **D189**
o-phenylene dichloride **D188**
p-phenylene dichloride **D190**
p-phenylenediisopropylidene bis(*tert*-butyl peroxide) **D154**
 1,4-phenylenediisothiocyanic acid **B138**
 1,10-(*o*-phenylene)pyrene **I24**
o-phenylenepylene **I24**
 phenylene thiocyanate **B138**
o-phenylenethiourea **M60**
 phenylephrine **P106**
 phenylethane **E97**
 1-phenylethanol **P68**
 2-phenylethanol **P67**
 2-phenylethanol acetate **P66**
 1-phenylethanone **A21**
 phenylethene **S126**
 phenyl ether **D544**
 2-phenylethyl acetate **P66**
 1-phenylethyl alcohol **P68**
 2-phenylethyl alcohol **P67**
 2-phenylethylamine **P69**
 phenylethyl ethanoate **P66**
 phenyl ethyl ether **P73**
 5-phenyl-5-ethylhexahydropyrimidine-4,6-dione **P272**
 β -phenylethylhydrazine **P65**
 β -phenylethylhydrazine sulfate **P64**
N-(2-phenylethyl)imidodicarbonimidic diamide **P74**
 (2-phenylethyl isothiocyanate)benzene **P70**
 phenylfluoroform **B80**
 phenylformic acid **B63**
 phenyl glycidyl ether **G35**
 (6*R*)-6-(α -D-phenylglycylamino)penicillanic acid **A194**
 phenylglyoxylonitrile oxime *O,O*-diethyl phosphorothioate **P170**
N-phenyl-*N'*-guanylguanidine **P95**
 1-phenylhexane **P107**
 phenylhydrazine **P108**
 phenylhydrazine **P109**
 2-phenylhydrazinecarboxamide **P75**
 phenylhydrazine hydrochloride **P109**
N-phenylhydrazine hydrochloride **P109**
 phenyl hydride **B47**
 phenylhydroquinone **P110**
 phenyl 2-hydroxybenzoate **P132**
 phenylhydroxymercury **P119**
 phenylic acid **P80**
 1-phenylimidazole **P111**
 1-phenyl-1H-imidazole **P111**
N-phenylimidazole **P111**
 2-phenyl-2-imidazoline **P112**
 phenylimide **P175**
N-phenylimidodicarbonimidic diamide **P95**
 phenyl iodide **I45**
 phenyl isocyanate **P113**
 phenyl isocyanate formaldehyde polymer **P114**
 2-phenylisopropanol **P131**
 (phenylisopropyl)amine **A193**
 phenyl isothiocyanate **P115**
 phenylmercaptan **B50**
 phenylmercuric acetate **P116**
 phenylmercuric borate **P117**
 phenylmercuric chloride **P118**
 phenylmercuric hydroxide **P119**
 phenylmercuric nitrate, basic **P120**
 phenylmercury acetate **P116**
 phenylmercury(II) borate **P117**
 phenylmercury(II) chloride **P118**
 phenylmercury(II) hydroxide **P119**
 phenylmercury(II) nitrate **P120**
 phenylmethane **T173**

phenylmethanol **B89**
 phenylmethylamine **B90**
N-phenylmethylamine **M156**
 1-phenyl-2-methylaminopropanol sulfate **E31**
 phenylmethyldichlorosilane **D224**
N-(phenylmethyl)dimethylamine **D403**
S-(phenylmethyl) dipropylidicarbamothioate **P340**
 phenyl methyl ether **A216**
 phenyl methyl ketone **A21**
 1-phenyl-3-methyl-5-pyrazolone **P121**
 phenyl mustard oil **P115**
N-phenyl-2-naphthalenamine **P124**
 phenylnaphthalene **P122**
 2-phenylnaphthalene **P123**
 β -phenylnaphthalene **P123**
 2-phenyl-4*H*-naphtho[1,2-*b*]pyran-4-one **N13**
 3-phenyl-1*H*-naphtho[2,1-*b*]pyran-1-one **N14**
N-phenyl-2-naphthylamine **P124**
N-phenyl- β -naphthylamine **P124**
N-phenyl-*p*-nitrosoaniline **N154**
 phenyloxirane **S127**
 phenyl oxirane **S127**
 3-phenyloxy-1,2-epoxypropane **G35**
 2-phenylphenol **P125**
 3-phenylphenol **P126**
 4-phenylphenol **P127**
o-phenylphenol **P125**
p-phenylphenol **P127**
 2-phenylphenol, sodium salt **S86**
o-phenylphenol, sodium salt **S86**
N-phenyl-*p*-phenylenediamine **P128**
 phenylphosphine **P129**
 phenylphosphine dichloride **D242**
 phenyl phosphite **T339**
 phenylphosphonous acid dichloride **D242**
 phenylphosphonous dichloride **D242**
N-phenylphthalamic acid **P130**
 phenyl phthalate **D549**
 1-phenylpropane **P324**
 2-phenylpropane **C474**
 2-phenyl-2-propanol **P131**
 phenylpropanolamine hydrochloride **N203**
 2-phenyl-2-propenal **C346**
 3-phenylpropenal **C346**
 2-phenylpropene **M307**
 3-phenyl-2-propenyl anthranilate **C347**
 3-phenyl-2-propen-1-yl anthranilate **C347**
 3-phenyl-2-propenyl propionate **C349**
 6-phenyl-2,4,7-pteridinetriamine **T203**
 1-phenyl-3-pyrazolidinone **P76**
 1-phenyl-2-pyrazolin-3-ol **P76**
N'-(1-phenylpyrazol-5-yl)sulfanilamidopyrazole **S139**
 phenyl-(2-pyridyl methyl)- β -(*N,N*-dimethylamino)ethyl ether **D598**
 phenyl salicylate **P132**
 1-phenylsemicarbazide **P75**
 phenylsilatrane **P133**
 1-phenylsilatrane **P133**
 phenylsilicon trichloride **P137**
 phenyl sulfohydrazide **B49**
 phenyl sulfone **P134**
 phenylsulfonyl chloride **B48**
 phenylsulfonyl hydrazide **B49**
 phenyl sulfoxide **P135**
 phenylthiocarbamide **P136**
 phenyl thioisocyanate **P115**
 phenylthiourea **P136**
 1-phenylthiourea **P136**
 1-phenyl-2-thiourea **P136**
 α -phenylthiourea **P136**
N-phenylthiourea **P136**
 phenyltoluene **M168**
 2-phenyltoluene **M169**
 4-phenyltoluene **M170**
 1-phenyl-1,2,4-triazolyl-3-(*O,O*-diethyl thionophosphate) **T205**
 phenyltrichlorosilane **P137**
 phenyltrimethylammonium chloride **P138**
 phenyltrimethylammonium iodide **P139**
 1-phenyl-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane **P133**
 phenylamidol **P140**
 phenytoin **P141**
 phenytoin sodium **P142**
 phenzidol **P143**
 phenzidole **P143**
 Philips-Duphar U-101 **T98**
 Philocap **C59**
 PhIP **P144**
 Phlogont (salve) **G38**
 phlorol **E160**
 phloxinrhodamine **C396**
 Phob **P79**
 pholate **A229**
 phorate **P145**
 phorbol **P146**
 4 β -phorbol **P146**
 phorone **P147**
 phosacetim **P148**
 phosalone **P149**
 Phoschlor **T225**
 phosdiphen **P150**
 Phosdrin **M330**
 Phosethyl Al **F108**
 Phosfleur **C309**
 Phosflex TPP **T337**
 phosfolan **P151**
 phosgen **P152**
 phosgene **P152**
 phosmet **P153**
 phosphacol **P10**
 phosphamidon **P154**
 phosphamidone **P154**
 phosphine **P155**

1,1',1''-phosphinylidynetrisaziridine **T346**
 1,1',1''-phosphinylidynetris(2-methylaziridine) **M99**
 phosphofluoridic acid **F71**
 phospholan **P151**
 phosphonadithioimidocarbonic acid, cyclic propylene *P,P*-diethyl ester **M56**
 phosphonic acid, 2-chloroethyl- **E63**
N-(phosphonomethyl)glycine **G40**
 phosphonothioic acid, (1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)-, *O,O*-diethyl ester **D569**
 phosphonothioic acid, methyl-, *O*-ethyl *O*-[*p*-(methylthio)-phenyl] ester **E150**
 phosphonothioic acid, phthalimido-, *O,O*-diethyl ester **D569**
 phosphoramidic acid, methyl-, 2-chloro-4-(1,1-dimethylethyl)phenylmethyl ester **C471**
 phosphoric acid **P156**
 phosphoric acid, bis(2,4-dichlorophenyl)ethyl ester **P150**
 phosphoric acid, butyl ester **B237**
 phosphoric acid, 2-chloro-1-(2,4-dichlorophenyl)ethenyl diethyl ester **C128**
 phosphoric acid, 2-chloro-3-(diethylamino)-1-methyl-3-oxo-1-propenyl dimethyl ester **P154**
 phosphoric acid, 2-chloro-1-(2,4,5-trichlorophenyl)ethenyl dimethyl ester, (*Z*)- **T60**
 phosphoric acid, 1,2-dibromo-2,2-dichloroethyl dimethyl ester **N3**
 phosphoric acid, 2,3-dibromopropyl ester **T352**
 phosphoric acid, dibutyl ester **D147**
 phosphoric acid, dibutyl phenyl ester **D159**
 phosphoric acid, 2,2-dichloroethenyl dimethyl ester **D258**
 phosphoric acid, diethyl 5-methyl-1*H*-pyrazol-3-yl ester **D311**
 phosphoric acid, diethyl 4-nitrophenyl ester **P10**
 phosphoric acid, dimethyl ester, ester with 2-chloro-*N,N*-diethyl-3-hydroxycrotonamide **P154**
 phosphoric acid, *O,O*-dimethyl *O*-[2-(ethylthio)ethyl] ester **D50**
 phosphoric acid, dimethyl *p*-(methylthio)phenyl ester **M311**
 phosphoric acid, lead(2+) salt (2:3) **L27**
 phosphoric acid, 4-(methylthio)phenyl dipropyl ester **P298**
 phosphoric acid, *p*-(methylthio)phenyl dipropyl ester **P298**
 phosphoric acid, sodium salt (1:3) **T359**
 phosphoric acid triethylene imide **T346**
 phosphoric acid, triethyl ester **T287**
 phosphoric acid, trimethyl ester **T324**
 phosphoric acid, trioctyl ester **T332**
 phosphoric acid, tris(2-ethylhexyl) ester **T355**
 phosphoric acid, tris(methylphenyl) ester **T361**
 phosphoric acid, tris(2-methylphenyl) ester **T362**
 phosphoric acid, tri-*o*-tolyl ester **T362**
 phosphoric anhydride **P163**
 phosphoric chloride **P160**
 phosphoric sulfide **P162**
 phosphorochloridic acid, diethyl ester **D299**
 phosphorochloridithioic acid, *O,O*-diethyl ester **D300**
 phosphorodiamidic acid, *N,N*-bis(2-chloroethyl)-*N'*-(3-hydroxypropyl), cyclohexylamine salt **C548**
 phosphorodiethioic acid, *S*-[[[1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)methyl] *O,O*-dimethyl] **P153**
 phosphorodithioic acid, *S*-chloromethyl *O,O*-diethyl ester **C140**
 phosphorodithioic acid, *S*-[(6-chloro-2-oxo-3(2*H*)-benzoxazolyl)methyl] *O,O*-diethyl ester **P149**
 phosphorodithioic acid, *S*-[[[4-chlorophenyl]thio]methyl] *O,O*-diethyl ester **C82**
 phosphorodithioic acid, *S*-[(4,6-diamino-1,3,5-triazin-2-yl)methyl] *O,O*-dimethyl ester **M50**
 phosphorodithioic acid, *S*-[(4,6-diamino-*s*-triazin-2-yl)methyl] *O,O*-dimethyl ester **M50**
 phosphorodithioic acid, *O*-(2,4-dichlorophenyl) *O*-ethyl *S*-propyl ester **P341**
 phosphorodithioic acid, *S*-[[[2,5-dichlorophenyl]-thio]methyl] *O,O*-diethyl ester **P77**
 phosphorodithioic acid, *O,O*-diethyl ester, *S*-ester with 6-chloro-3-(mercaptomethyl)-2-benzoxazolinone **P149**
 phosphorodithioic acid, *O,O*-diethyl ester, *S*-ester with *N*-isopropyl-2-mercaptoacetamide **P342**
 phosphorodithioic acid, *O,O*-diethyl *S*-[2-ethylsulfanyl]-ethyl] ester **D567**
 phosphorodithioic acid, *O,O*-diethyl *S*-[(ethylthio)methyl] ester **P145**
 phosphorodithioic acid, *O,O*-diethyl *S*-[2-[(1-methylethyl)amino]-2-oxoethyl] ester **P342**
 phosphorodithioic acid, *O,O*-diisopropylester *S*-ester with *N*-(2-mercaptoethyl)benzenesulfonamide **B36**
 phosphorodithioic acid, *O,O*-dimethyl ester, *S*-ester with 4-(mercaptoacetyl)morpholine **M354**
 phosphorodithioic acid, *O,O*-dimethyl ester, *S*-ester with 2-mercapto-*N*-methylacetamide **D376**
 phosphorodithioic acid, *O,O*-dimethyl ester, *S*-ester with *N*-(mercaptomethyl)phthalimide **P153**
 phosphorodithioic acid, *S*-[2-(ethylamino)-2-oxoethyl] *O,O*-dimethyl ester **E71**
 phosphorodithioic acid, *S,S*-methylene, *O,O,O',O'*-tetraethyl ester **E68**
 phosphorodithioic acid, *O,O*-dimethyl *S*-[2-(4-morpholinyl)-2-oxoethyl]ester **M354**
 phosphorofluoridic acid, bis(1-methylethyl) ester **I106**
 phosphorofluoridic acid, diisopropyl ester **I106**
 phosphorofluoridic acid, disodium salt **D563**
 phosphoromidothioic acid, 1-methylpropyl-, *O*-ethyl *O*-(5-methyl-2-nitrophenyl) ester **B198**
 phosphorothioic acid **D167**
 phosphorothioic acid, *S*-benzyl *O,O*-diisopropyl ester **I61**
 phosphorothioic acid, *O,O*-bis(1-methylethyl) *S*-(phenylmethyl) ester **I61**
 phosphorothioic acid, *O*-(4-bromo-2,5-dichlorophenyl)-, *O,O*-diethyl ester **B184**
 phosphorothioic acid, *O*-(4-bromo-2,5-dichlorophenyl)-, *O,O*-dimethyl ester **B183**
 phosphorothioic acid chloride **T141**

phosphorothioic acid, *O*-(3-chloro-4-nitrophenyl) *O,O*-dimethyl ester **C320**
 phosphorothioic acid, *S*-[2-[(1-cyano-1-methylethyl)amino]-2-oxoethyl] *O,O*-diethyl ester **C490**
 phosphorothioic acid, *O*-(4-cyanophenyl) *O,O*-dimethyl ester **C486**
 phosphorothioic acid, cyclic *O,O*-(methylene-*o*-phenylene) *O*-methyl ester **D527**
 phosphorothioic acid, *O*-(2,5-dichloro-4-iodophenyl) *O,O*-dimethyl ester **I50**
 phosphorothioic acid, *O*-[2,5-dichloro-4-(methylthio)-phenyl] *O,O*-diethyl ester **C321**
 phosphorothioic acid, *S*-[2-(diethylamino)ethyl]-, *O,O*-diethyl ester, oxalate **A157**
 phosphorothioic acid, *O*-[2-(diethylamino)-6-methyl-4-pyrimidinyl] *O,O*-dimethyl ester **P210**
 phosphorothioic acid, *O,O*-diethyl ester, *S*-ester with *N*-(1-cyano-1-methylethyl)-2-mercaptoacetamide **C490**
 phosphorothioic acid, *O,O*-diethyl *S*-[2-ethylsulfonyl]ethyl ester **D56**
 phosphorothioic acid, *O,O*-diethyl *O*-[2-(ethylthio)ethyl] ester **D51**
 phosphorothioic acid, *O,O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester **D99**
 phosphorothioic acid, *O,O*-diethyl *O*-(4-methyl-2-oxo-2*H*-1-benzopyran-7-yl) ester **D309**
 phosphorothioic acid, *O,O*-diethyl *O*-[(*p*-methylsulfinyl)-phenyl] ester **F23**
 phosphorothioic acid, *O,O*-diethyl *O*-(*p*-nitrophenyl) ester **P13**
 phosphorothioic acid, *O,O*-diethyl *O*-(5-phenyl-3-isoxazolyl) ester **I143**
 phosphorothioic acid, *O,O*-diethyl *O*-pyrazinyl ester **T135**
 phosphorothioic acid, *O*-[4-[(dimethylamino)sulfonyl]-phenyl] *O,O*-dimethyl ester **F1**
 phosphorothioic acid, *O,O*-dimethyl ester, *S*-ester with 2-mercapto-*N*-methylacetamide **O32**
 phosphorothioic acid, *O,O*-dimethyl *O*-*p*-hydroxy-*N,N*-dimethylbenzenesulfonamide ester **F1**
 phosphorothioic acid, *O,O*-dimethyl *O*-(3-methyl-4-nitrophenyl) ester **F11**
 phosphorothioic acid, *O,O*-dimethyl *O*-[4-(methylthio)-*m*-tolyl] ester **F24**
 phosphorothioic acid, *S*-[2-(ethylsulfinyl)ethyl] *O,O*-dimethyl ester **O57**
 phosphorothioic acid, *O*-methyl ester, cyclic *O,O*-ester with *o*-hydroxybenzyl alcohol **D527**
 phosphorothionic acid trichloride **T141**
 phosphorotrithious acid, tributyl ester **M89**
 phosphorous acid **P157**
 phosphorous acid, dimethyl ester **D449**
 phosphorous acid, triethyl ester **T288**
 phosphorous acid, trimethyl ester **T325**
 phosphorous acid, triphenyl ester **T339**
 phosphorus **P158**
 phosphorus, black **P158**
 phosphorus bromide **P165**
 phosphorus chloride **P166**
 phosphorus(III) oxide **P167**
 phosphorus(V) oxide **P163**
 phosphorus oxychloride **P159**
 phosphorus pentachloride **P160**
 phosphorus pentafluoride **P161**
 phosphorus pentasulfide **P162**
 phosphorus pentoxide **P163**
 phosphorus perchloride **P160**
 phosphorus persulfide **P162**
 phosphorus, red **P158**
 phosphorus sesquisulfide **P164**
 phosphorus sulfide **P164**
 phosphorus sulfochloride **T141**
 phosphorus thiochloride **T141**
 phosphorus tribromide **P165**
 phosphorus trichloride **P166**
 phosphorus trihydride **P155**
 phosphorus trioxide **P167**
 phosphorus, white **P158**
 phosphorus, yellow **P158**
 phosphoryl chloride **P159**
 phosphoryl oxytrichloride **P159**
 phosphothion **M11**
 Phostoxin **A104**
 Phosvel **L35**
 Phosvin **Z14**
 photodiethyl **P168**
 Photodyns **H13**
 photomirex **P169**
 Photozinc **Z12**
 phoxim **P170**
 PHT **P139**
 Phthalophos **P153**
 phthalamide **P171**
 1,3-phthalandione **P173**
 phthalanilic acid **P130**
 1(2*H*)-phthalazinone hydrazone hydrochloride **H85**
 phthaldiamide **P171**
 phthalic acid **P172**
m-phthalic acid **I113**
o-phthalic acid **P172**
p-phthalic acid **T26**
 phthalic acid, benzyl butyl ester **B94**
 phthalic acid, butyl ester **M341**
 phthalic acid diamide **P171**
 phthalic acid, dibutyl ester **D160**
 phthalic acid, dicyclohexyl ester **D268**
 phthalic acid, didecyl ester **D275**
 phthalic acid, diisobutyl ester **D354**
 phthalic acid, monobutyl ester **M341**
 phthalic acid, mono(2-ethylhexyl) ester **M344**
 phthalic acid, mono-octyl ester **M346**
 phthalic acid, monopentyl ester **M347**
 phthalic anhydride **P173**
o-phthalic anhydride **P173**
 phthalic anhydride, 1,2,3,6-tetrahydro- **T76**

o-phthalic imide **P175**
 phthalic monoanilide **P130**
 phthalide **P174**
 phthalimide **P175**
 2-phthalimidoglutarimide **T99**
 (SP-4-1)-[29*H*,31*H*-phthalocyaninato (2-)-*N*²⁹,*N*³⁰,*N*³¹,*N*³²]-copper **P176**
 phthalocyanine blue **P176**
m-phthalodinitrile **I114**
 (phthaloyldioxy)bis[tributyltin **T220**
N-phthaloylglutarimide **T99**
 phthalthrin **T85**
 2-(*N*⁴-phthalylaminobenzenesulfonamido)thiazole **P177**
 phthalylsulfathiazole **P177**
 phthalylsulfonazole **P177**
 phylloquinone **P181**
 physostal salicylate **P179**
 physostigmine **P178**
 physostigmine salicylate **P179**
 Phytosol **P178**
 Phytar **C1**
 phytic acid **P180**
 phytolaccanin **B107**
 phytomenadione **P181**
 phytonadione **P181**
 Phytosol **T253**
 phytylmenaquinone **P181**
 PIA **I113**
 Pichtosin **I83**
 Pichtosine **I83**
 picloram **P182**
 2-picoline **P183**
 3-picoline **P184**
 4-picoline **P185**
 α-picoline **P183**
 β-picoline **P184**
 γ-picoline **P185**
m-picoline **P184**
o-picoline **P183**
p-picoline **P185**
 picolinic acid, 3,6-dichloro- **C364**
 picolinonitrile **C487**
 2-picolyl chloride hydrochloride **P186**
 picramic acid **A126**
 picrate of ammonia **A182**
 picric acid **P187**
 picrite (the explosive) **N122**
 picronitric acid **P187**
 picrotoxin **P188**
 picrylmethylnitramine **N65**
 pigment lake red BFC **D27**
 Pigment Red 23 **C417**
 Pigment Red 3 **C416**
 pigment red barium salt (53:1) **D27**
 Pi Habs **C34**
 Pilargon **P315**
 Pilartex **F24**
 Pillarsete **B196**
 pilocarpine **P189**
 (+)-pilocarpine **P189**
 pilocarpine chloride **P190**
 pilocarpine hydrochloride **P190**
 pilocarpine, monohydrochloride **P190**
 pilocarpine muriate **P190**
 pilocarpinium chloride **P190**
 pilocarpol **P189**
 Pimafucin **P191**
 pimaricin **P191**
 pimelic ketone **C509**
 pinacolin **P192**
 pinacolone **P192**
 pindone **P193**
 (+)-2-pinene **P196**
 (+)-α-pinene **P196**
 (1*R*,5*R*)-(+)-2-pinene **P196**
 (1*R*)-(+)-α-pinene **P196**
 (1*S*,5*S*)-(-)-2-pinene **P194**
 (1*S*)-(-)-α-pinene **P194**
 (1*S*)-(-)-β-pinene **P199**
 2-pinene **P195**
 2(10)-pinene **P198**
 α-pinene **P195**
 β-pinene **P198**
 L-β-pinene **P199**
 (-)-pinene **P194**
 (±)-2-pinene **P197**
 (±)-α-pinene **P197**
 Pinofon **T63**
 Pinulin **V23**
 piperazine **P200**
 piperazine **P200**
 1-piperazinecarboxamide, *N,N*-diethyl-4-methyl-, 2-hydroxy-1,2,3-propanetricarboxylate (1:1) **D295**
 piperazine, 1-[(4-chlorophenyl)phenylmethyl]-4-methyl-, hydrochloride **C188**
N,N'-[1,4-piperazinediylbis (2,2,2-trichloroethylidene)]bisformamide **T295**
 piperidine **P201**
 2,6-piperidinedicarboxylic acid 4-[2-[2-carboxy-5-(β-D-glucopyranosyloxy)-2,3-dihydro-6-hydroxy-1*H*-indol-1-yl]ethylidene **B25**
 2-piperidinone **P202**
 2-piperidone **P202**
 piperine **P203**
 piperonal bis[2-(2-butoxyethoxy)ethyl]acetal **P207**
 piperonyl butoxide **P204**
 piperonyl sulfoxide **S148**
 piperophos **P205**
 1-piperoylpiperidine **P203**
 piproctanyl bromide **P206**
 piprotal **P207**
 Piria's acid **A132**
 Pirimal **S132**
 pirimicarb **P208**

pirimiphos-ethyl **P209**
 pirimiphos-methyl **P210**
 Pirimor **P208**
 Piristin **T334**
 pirivatol **P358**
 Pirmazin **S133**
 pirod **U8**
 pitch, coal tar **C367**
 Pittchlor **C34**
 Pivacin **P193**
 Pival **P193**
 pivaldione **P193**
 pivalic acid lactone **P211**
 pivalolactone **P211**
 2-pivaloylindan-1,3-dione **P193**
 2-pivalyl-1,3-indandione **P193**
 Pivalyl Valone **P193**
 Pivot **I7**
 Pivot **I6**
 Planavin **N64**
 Planete **H43**
 Planofix **N22**
 Plantonit **T25**
 Plant Pin **B225**
 Plantvax **O56**
 Planuin **N64**
 plastikator BA **D120**
 Plastomoll BMB **B248**
 platinic ammonium chloride **A170**
 platinic chloride **C261**
 Platinol **C350**
 platinum chloride **P213**
 platinum **P212**
 platinum black **P212**
 platinum(II) chloride **P213**
 platinum(IV) chloride **P214**
 platinum dichloride **P213**
 cis-platinum II **C350**
 platinum sponge **P212**
 platinum tetrachloride **P214**
 Platistin **C350**
 playdax **T22**
 plifenate **P215**
 Pliviol E **P225**
 Plondrel **D569**
 plumbagin **P216**
 Plumbagine **P216**
 plumbago **G45**
 plumbic acetate **L32**
 plumbic oxide **L19**
 plumbous chloride **L15**
 plumbous chromate **L16**
 plumbous fluoride **L22**
 plumbous iodide **L24**
 plumbous nitrate **L25**
 plumbous sulfide **L31**
 Pluronic L-81 **P218**
 Pluronic L44 **P218**
 PMB **P117**
 PMC **P118**
 PMDA **P364**
 PMF (antioxidant) **M144**
 PMP **P153**
 PMS artificial tears **P234**
 PNB **N100**
 PO **P330**
 Podigrol **P360**
 podocarpa-7,13-dien-15-oic acid, 13-isopropyl- **A2**
 Polaris **G41**
 Polikarbacin **M321**
 polixetonium chloride **P217**
 Pollux **Z14**
 Poloxalcol **P218**
 poloxalene **P218**
 poloxamer **P218**
 Poltan **B142**
 Polybor **B141**
 Polybrene **I56**
 polybrominated biphenyls **P219**
 polybrominated salicylanilide **T208**
 polychlorinated biphenyl **A238**
 polychlorinated biphenyl **A239**
 polychlorinated biphenyl **A233**
 polychlorinated terphenyls **P220**
 polychlorocamphene **C48**
 polychloroterpenes **P221**
 Polycillin **A194**
 Polycycline **T62**
 poly(1,2-dihydro-2,2,4-trimethylquinoline) **A16**
 poly[(dimethylimino)hexamethylene(dimethylimino)trimethylene]dibromide **I56**
 polydimethylsiloxane **P222**
 Polydis TR 131 **E46**
 polyestradiol phosphate **P223**
 polyethene **P224**
 polyethylene **P224**
 polyethylene glycol **P225**
 poly(ethylene glycol) **P225**
 polyethylene glycol mono(nonylphenyl) ether **N196**
 polyethylene glycol mono(4-octylphenyl) ether **O20**
 polyethylene glycol sorbitan monolaurate **P227**
 polyethylene glycol sorbitan monooleate **P230**
 polyethylene glycol sorbitan monopalmitate **P228**
 polyethylene glycol sorbitan monostearate **P229**
 polyethylene oxide **P225**
 polyethylene-polypropylene glycol **P218**
 poly(ethylene tetrafluoride) **P232**
 polyglycol 200 **P225**
 polyglycol 300 **P225**
 Polylin 515 **L49**
 polymeric MDI **P114**
 polymers acetic acid vinyl ester **P233**
 poly(methylene phenylene isocyanate) **P114**
 polymethylene polyphenyl isocyanate **P114**

polymethyl methacrylate **P226**
 Polymox **A192**
 polyoestradiol phosphate **P223**
 polyox **P225**
 poly[1-(2-oxo-1-pyrrolidinyl)ethylene] **P236**
 poly[oxy(dimethylsilylene)] **P222**
 poly(oxy-1,2-ethanediyl), α -(4-nonylphenyl)- ω -hydroxy-**N196**
 poly(oxy-1,2-ethanediyl) sorbitan monooctadecanoate **P229**
 polyoxyethylene **P225**
 polyoxyethylene derivatives sorbitan monopalmitate **P228**
 poly[oxyethylene(dimethylimino)ethylene(dimethylimino)ethylene]dichloride **P217**
 poly(oxyethylene)glycol **P225**
 polyoxyethylene mono-*p*-nonylphenyl ether **N196**
 poly(oxyethylene)*p*-*tert*-octylphenyl ether **O20**
 polyoxyethylene (20) sorbitan monolaurate **P227**
 polyoxyethylene (20) sorbitan monooleate **P230**
 poly(oxyethylene) sorbitol monostearate **P229**
 Polypodine A **E1**
 Polyram **M321**
 Polysect **B109**
 Poly-solv DM **M135**
 Polysolv EE **E76**
 Poly-solv EE acetate **E79**
 Poly-Solv PPM **D556**
 polysorbate 20 **P227**
 polysorbate 40 **P228**
 polysorbate 60 **P229**
 polysorbate 80 **P230**
 polystyrene **P231**
 Polytanol **C41**
 polytef **P232**
 polytetrafluoroethylene **P232**
 Polythanol **C41**
 Polythene **P224**
 Polyvel PLC-20 **D264**
 polyvidone **P236**
 polyvinyl acetate **P233**
 polyvinyl alcohol **P234**
 polyvinyl chloride **P235**
 polyvinylpyrrolidone **P236**
 polyviol **P234**
 Polywax 1000 **P224**
 Pomalus Acid **M15**
 Pomarsol Z **Z19**
 Ponceau MX **C395**
 Ponceau 2R **C395**
 Ponceau 3R **C414**
 Ponceau 4R **C394**
 Ponceau Red **C395**
 Ponstan **M42**
 Ponstil **M42**
 Pontamine Fast Blue 7GLN **C406**
 Porcelain clay **K2**
 Porofo 57 **A269**
 Portland cement silicate **C99**
 Portland stone **C25**
 Posse **C83**
 Potablan **M340**
 potassa **P254**
 potassium **P237**
 potassium acid arsenate **P238**
 potassium acid fluoride **P252**
 potassium acid sulfate **P253**
 potassium alum **A105**
 potassium antimonyl tartrate **A222**
 potassium arsenate **P238**
 potassium arsenite **P239**
 potassium bichromate **P246**
 potassium bifluoride **P252**
 Potassium bis(cyano-C)-argenate(1-) **P262**
 potassium bis(2-hydroxyethyl)dithiocarbamate **P240**
 potassium bisulfate **P253**
 potassium bromate **P241**
 potassium chlorate **P242**
 potassium chloride **P243**
 potassium chromate **P244**
 potassium chromate(vi) **P244**
 potassium cyanide **P245**
 potassium cymonate **P249**
 potassium dichromate **P246**
 potassium dichromate(vi) **P246**
 potassium dicyanoargenate **P262**
 potassium dimethyldithiocarbamate **P247**
 potassium dioxide **P265**
 potassium ethylenediaminetetraacetate **E6**
 potassium fluoride **P248**
 potassium fluoroacetate **P249**
 potassium fluorosilicate **P250**
 potassium fluoro-zirconate(iv) **P251**
 potassium fluozirconate **P251**
 potassium 2,4-hexadienoate **P263**
 potassium hexafluorosilicate **P250**
 potassium hexafluoro-zirconate **P251**
 potassium hydrate **P254**
 potassium hydrogen arsenate **P238**
 potassium hydrogen difluoride **P252**
 potassium hydrogen fluoride **P252**
 potassium hydrogen sulfate **P253**
 potassium hydroxide **P254**
 potassium hyperchloride **P259**
 potassium iodate **P255**
 potassium iodide **P256**
 potassium iodine oxide **P255**
 potassium iodohydrargyrate **P266**
 potassium mercuric iodide **P266**
 potassium metaarsenite **P239**
 potassium nitrate **P257**
 potassium nitrite **P258**
 potassium oxymuriate **P242**
 potassium perchlorate **P259**

potassium permanganate **P260**
 potassium peroxydisulfate **P261**
 potassium persulfate **P261**
 potassium silicofluoride **P250**
 potassium silver cyanide **P262**
 potassium sorbate **P263**
 potassium sulfate **P264**
 potassium superoxide **P265**
 potassium tetraiodomercurate(II) **P266**
 potavescent **P243**
 potcrate **P242**
 povidone **P236**
 POX **P163**
 PP 062 **P208**
 PP 333 **P1**
 PP 511 **P210**
 PPTC **V19**
 pracarbamin **U13**
 prallethrin **P267**
 pralléthrine **P267**
 praseodymium **P268**
 Prazepine **I14**
 Prebane **T25**
 Precipite blanc **M70**
 Precision **F17**
 Predict **N206**
 prednisolone **P269**
 prednisolone F **D62**
 Prefar **B36**
 Prefix **C319**
 1,4-pregnadione-3,20-dione-11 β ,17 α ,21-triol **P269**
 pregn-4-ene-21-carboxylic acid, 7-(acetylthio)-17-hydroxy-3-oxo, γ -lactone, (7 α ,17 α) **S108**
 pregn-4-ene-3,20-dione **P282**
 4-pregnen-17 α -ol-3,20-dione **H115**
 pregnenolone **P270**
 Δ^5 -pregnon-3 β -ol-20-one **P270**
 Premier **I8**
 Premise **I8**
 Prenazone **F29**
 Prenimon **T345**
 Prenol **M176**
 Prentox **P204**
 prenyl alcohol **M176**
 prenylamine **P271**
 Prep **E63**
 Pre-san **B36**
 Presinol **M208**
 Preventol **D235**
 Preventol A3 **D217**
 Preventol I **T258**
 Previson **N205**
 Pride **F86**
 Pride **F6**
 Primaclone **P272**
 primary amyl acetate **A195**
 Primatol P **P302**
 Prime **F45**
 Primicid **P209**
 primidone **P272**
 primidos **N207**
 Primotec **P209**
 Prince **F33**
 Principen **A194**
 Prinolutin **N204**
 Prinsyl **D256**
 Probe **M120**
 Probeltion **E68**
 procaine **P273**
 procarbazine **P274**
 Procarbazine hydrochloride **I1**
 prochloraz **P275**
 prochlorpemazine **P276**
 prochlorperazine **P276**
 prochlorpromazine **P276**
 Procidin S 735A **P50**
 proconazole **P306**
 procymidone **P277**
 Prodan **S68**
 Prodex **M111**
 prodiamine **P278**
 Prodox **H115**
 Productol **C456**
 Profenid **K10**
 profenofos **P279**
 proflavine hydrochloride **P280**
 proflavin hydrochloride **P280**
 profluorane **O7**
 profluralin **P281**
 Progallin **P332**
 progesterone **P282**
 proglinazine-ethyl **P283**
 Prograss **E72**
 Pro-Gro **C84**
 Prolate **P153**
 L-proline **P284**
 promazine hydrochloride **P285**
 promecarb **P286**
 Promet **F125**
 promethazine **P287**
 prometron **P288**
 prometone **P288**
 prometryn **P289**
 promoteston **T38**
 pronamide **P339**
 propachlor **P290**
 propachlore **P290**
 Propacil **P337**
 propaldehyde **P309**
 propamide **P295**
 propamine D **T89**
 propamocarb hydrochloride **P291**
 propanal **P309**
 n-propanal **P309**

propanamide, *N*-ethyl-2-[(phenylamine)carbonyl]-oxy)-(R)- **C66**
 1-propanamine **P323**
 2-propanamine **I121**
 1-propanamine, 3-(10,11-dihydro-5*H*-dibenzo(a,d)cyclohepten-5-ylidene, *N,N*-dimethyl- **A159**
 propane **P292**
 1-propanecarboxylic acid **B285**
 1,3-propanedial **M16**
 1,3-propanedialdehyde **M16**
 1,2-propanediamine **D83**
 1,3-propanediamine **D84**
 propanedinitrile **M18**
 propanedioic acid **M17**
 propanedioic acid, dithallium salt **T105**
 1,2-propanediol **P327**
 1,2-propanediol 1-acrylate **H116**
 1,2-propanediol dinitrate **P329**
 1,3-propanedione **M16**
 propane, 1,1-[1,2-ethenediylbis(sulfonyl)]bis-*E*- **B135**
 propane, 2-iodo-2-methyl- **I54**
 propane-2-nitrate **I129**
 propanenitrile **P312**
n-propanenitrile **P312**
 propanenitrile, 2,2'-azobis(2-methyl)- **A269**
 propanenitrile, 3-chloro- **C274**
 propanenitrile, 2-hydroxy-2-methyl- **A18**
 α,γ -propane oxide **T309**
 propane, 2,2'-oxybis(1-chloro-) **D26**
 Propaneperoxoic acid, 2,2-dimethyl-, 1,1-dimethylethyl ester **B273**
 propaneperoxoic acid, 2-methyl-1,1-dimethyl ester **B272**
 1,3-propane sultone **P293**
 γ -propane sultone **P293**
 1-propanethiol **P294**
 1,2,3-propanetricarboxylic acid, 2-hydroxy- **C352**
 1,2,3-propanetricarboxylic acid, 2-hydroxy-, triethyl ester **T279**
 1,2,3-propanetriol **G25**
 1,2,3-propanetriol triacetate **T196**
 1,2,3-propanetriol trinitrate **G26**
 1,2,3-propanetriyl butanoate **T223**
 Propanex **P295**
 propanil **P295**
 propanoic acid **P310**
 propanoic acid, anhydride **P311**
 propanoic acid, butyl ester **B277**
 propanoic acid, 2,2-dichloro-, 2-(2,4,5-trichlorophenoxy)ethyl ester **T261**
 propanoic acid, ethyl ester **E165**
 propanoic anhydride **P311**
 propan-1-ol **P296**
 1-propanol **P296**
 2-propanol **P297**
n-propanol **P296**
 1-propanol, 2,3-dibromo-, phosphate (3:1) **T352**
 3-propanolide **P308**
 propanol, methoxy- **M146**
 2-propanone **A17**
 1-propanone, 2-(diethylamino)-1-phenyl-, hydrochloride **D316**
 propanoyl chloride **P313**
 propaphos **P298**
 propaquizafop **P299**
 Propardrine **N203**
 Propargil **P300**
 propargite **P300**
 propargyl alcohol **P301**
 propargyl chloride **C278**
 Propasol **M147**
 Propax **O48**
 propazine **P302**
 Propen **F14**
 prop-2-enal **A35**
 2-propenal **A35**
 propenal diethyl acetal **A39**
 propenamide **A41**
 2-propenamide **A41**
 2-propenamine **A74**
 2-propen-1-amine **A74**
 propene **P303**
 1-propene **P303**
 propene acid **A42**
 1-propene, 3-chloro- **A78**
 2-propene-1,1-diol diacetate **A37**
 2-propene-1,1-diyl bis(acetate) **A37**
 1-propene-2-methyl **I86**
 2-propenenitrile **A43**
 2-propenenitrile, 2-chloro- **C152**
 propene oxide **P330**
 1-propene trimer **T343**
 2-propenoic acid **A42**
 2-propenoic acid, 2,2-bis[(1-oxo-2-propenyl)oxy]methyl]-, 1,3-propanediyl ester **P36**
 2-propenoic acid, 1,4-butanediyl ester **B207**
 2-propenoic acid, 2,2-dimethyl-1,3-propanediyl ester **N41**
 2-propenoic acid, 1,6-hexanediyl ester **H61**
 2-propenoic acid, hexyl ester **H78**
 2-propenoic acid, 2-hydroxypropyl ester **H116**
 2-propenoic acid, 2-methyl-, oxiranylmethyl ester **G31**
 2-propenoic acid, 1-methyl-1,3-propanediyl ester **B206**
 2-propenoic acid, oxiranylmethyl ester **G29**
 2-propenoic acid, oxydi-2,4-ethanediyl ester **D302**
 2-propen-1-ol **A73**
 1-propen-2-ol acetate **I118**
 2-propen-1-ol, 3-phenyl-, formate **C348**
 2-propenoyl chloride **A44**
 propen-2-yl acetate **I118**
 2-propenylacrylic acid **S102**
 2-propenylamine **A74**
p-propenylanisole **A75**
 5-(1-propenyl)-1,3-benzodioxole **I136**
 5-(2-propenyl)-1,3-benzodioxole **S2**
 2-propenyl chloride **A78**

propenyl cinnamate **A80**
 4-propenylguaicol **I102**
 2-propenyl isothiocyanate **A87**
 2-propenyl isovalerate **A88**
 3-propenyl methanoate **A83**
 ((2-propenyloxy)methyl)oxirane **A84**
 1-(2-propenyloxy)propanol **P328**
 (2-propenyloxy)propanol **P328**
 2-propenyl phenylacetate **A91**
p-propenylphenyl methyl ether **A75**
N-2-propenyl-2-propen-1-amine **D70**
 2-propenyl propyl disulfide **A92**
 2-propenyl thiourea **A93**
 propetamphos **P304**
 propham **P305**
 Prophos **E74**
 propiconazole **P306**
 propine **P338**
 propineb **P307**
 1,3-propiolactone **P308**
 β -propiolactone **P308**
 propionaldehyde **P309**
 propionic acid **P310**
 propionic acid anhydride **P311**
 propionic acid, 2-(*N*-benzoyl-*N*-(3,4-dichlorophenyl)amino ethyl ester **B84**
 propionic acid chloride **P313**
 propionic acid, α -chloro- **C272**
 propionic acid, cinnamyl ester **C349**
 propionic acid, 2,2-dichloro-, 2-(2,4,5-trichlorophenoxy)ethyl ester **T261**
 propionic acid, isobutyl ester **I95**
 propionic acid, methyl ester **M290**
 propionic aldehyde **P309**
 propionic anhydride **P311**
 propionic chloride **P313**
 propionic ether **E165**
 propionic nitrile **P312**
 propionitrile **P312**
 propionyl chloride **P313**
 propionyl oxide **P311**
 propionyl peroxide **D552**
 propiophenone, 2-(diethylamino)-, hydrochloride **D316**
 propofol **P314**
 Propogon **P315**
 Propol **P297**
 propoxur **P315**
 2-propoxyethanol **P316**
 2-propoxyethanol acetate **P317**
 2-propoxyethyl acetate **P317**
 propoxyphene **P318**
l-propoxyphene **L39**
 propoxyphene-(+)- α -form **P318**
 propoxyphene(2*S*,3*R*)-form **P318**
 propoxyphene hydrochloride **P319**
 (+)-propoxyphene hydrochloride **P319**
 α -propoxyphene hydrochloride **P319**
 D-propoxyphene hydrochloride **P319**
 propoxyphene napsylate **P320**
 (+)-propoxyphene napsylate **P320**
 D-propoxyphene napsylate **P320**
 propranolol **P321**
 β -propranolol **P321**
 Proprasylyt **P321**
 propyl acetate **P322**
 propylacetic acid **V2**
 propyl alcohol **P296**
sec-propyl alcohol **P297**
 propylaldehyde **P309**
 propylamine **P323**
 2-propylamine **I121**
sec-propylamine **I121**
 propylbenzene **P324**
n-propylbenzene **P324**
 5-propyl-1,3-benzodioxole **D347**
 propyl bromide **B185**
 5-propyl butylethylthiocarbamate **P17**
 propyl carbamate **P325**
n-propyl carbamate **P325**
 5-propyl carbamothioate **V19**
 propylcarbinol **B212**
n-propylcarbonylchloride **B251**
 propyl cellosolve **P316**
 propyl chloride **C263**
 propyl chlorocarbonate **P326**
 propyl chloroformate **P326**
N-propyl-*N'*-*p*-chlorophenylsulfonylcarbamide **C311**
 propyl cyanide **B289**
 propyl *p,p'*-dichlorobenzilate **C276**
 5-propyl dipropylthiocarbamate **V19**
 propylene **P303**
 1-propylene **P303**
 propylenealdehyde **C467**
 propylene chloride **D245**
 propylene α -chlorohydrin **C266**
 propylene β -chlorohydrin **C267**
sec-propylene chlorohydrin **C266**
 propylenediamine **D83**
 propylenedicarboxylic acid **I144**
 propylene dichloride **D245**
 propylene dichlorohydrin **D247**
 propylene dinitrate **P329**
 propylene glycol **P327**
 propylene glycol allyl ether **P328**
 propylene glycol butoxy ether **B230**
 propylene glycol dinitrate **P329**
 1,2-propylene glycol dinitrate **P329**
 propylene glycol methyl ether acetate **M148**
 propylene glycol monoacrylate **H116**
 propylene glycol monoallyl ether **P328**
 propylene glycol monobutyl ether **B230**
 1,2-propylene glycol 1-monobutyl ether **B231**
 propylene glycol monomethyl ether **M146**
 propylene glycol monomethyl ether **M147**

propylene imine **M158**
 propylene nitrate **P329**
 propylene oxide **P330**
 1,2-propylene oxide **P330**
 1,3-propylene oxide **T309**
 propylenimine **M158**
 1,2-propylenimine **M158**
 propyl ether **D557**
 β -propyl- α -ethylacrolein **E125**
 propylethylene **P43**
 propyl ethyl ether **E82**
 propyl formate **P331**
 propylformic acid **B285**
 propyl gallate **P332**
 propyl glycol **P316**
 propyl hydride **P292**
 propyl 4-hydroxybenzoate **P336**
 propyl *p*-hydroxybenzoate **P336**
 propylic alcohol **P296**
 propylic aldehyde **P309**
 propylidene chloride **D244**
 propyl isocyanate **P333**
 1-propyl isocyanate **P333**
 propyl ketone **H25**
 propyl mercaptan **P294**
 propyl methanoate **P331**
 propyl methanoate **P322**
 propylmethanol **B212**
 4-propyl-1,2-(methylenedioxy)benzene **D347**
 propyl nitrate **P334**
 1-propyl-3-nitro-3-nitrosoguanidine **P335**
N-propyl-*N'*-nitro-*N*-nitrosoguanidine **P335**
 2-(propyloxy)ethanol **P316**
 propylparaben **P336**
 2-propylpentanoic acid **V8**
 6-propylpiperonyl butyl diethylene glycol ether **P204**
N-propyl-1-propanamine **D554**
 propyl thiol **P294**
 propyl thiopyrophosphate **T96**
 6-propyl-2-thiouracil **P337**
 1[*N*-propyl-*N*-[2-(2,4,6-trichlorophenoxy)ethyl]carbonyl]imidazole **P275**
N-propyl-*N*-[2-(2,4,6-trichlorophenoxy)ethyl]-1*H*-imidazole-1-carboxamide **P275**
 propyl 3,4,5-trihydroxybenzoate **P332**
 propyl urethane **P325**
 2-propylvaleric acid **V8**
 propylvinylcarbinol **H71**
 propyne **P338**
 1-propyne, 3-chloro- **C278**
 prop-2-yn-1-ol **P301**
 2-propynol **P301**
 2-propyn-1-ol **P301**
 3-propynol **P301**
 propynyl alcohol **P301**
 2-propynyl chloride **C278**
 propyzamide **P339**
 Prosthex **P234**
 prosulfocarb **P340**
 Protectol GDA **G21**
 Proterox **C319**
 prothiofos **P341**
 prothiophos **P341**
 prothoate **P342**
 Prothrombin **W3**
 protium **H96**
 protohematin **H12**
 Protol **H106**
 Protox **P233**
 Provado **I8**
 Proventil Inhaler **S3**
 Provitamin A **V40**
 provitamin D **E43**
 provitamin D₂ **E43**
 Prowl **P20**
 proxanol **P218**
 proxan-sodium **P343**
 Proxitane 4002 **P51**
 Prozac **F82**
 Prozinex **P302**
 Prulet **P81**
 prunetol **G9**
 Prussian red **I74**
 prussic acid **H100**
 Pryleugau **I15**
 pseudoacetic acid **P310**
 pseudobutyl benzene **B247**
 pseudobutylene **B216**
 pseudocumene **T307**
 pseudocumidine **T304**
 pseudocumol **T307**
 pseudocyanuric acid **C491**
 pseudohexyl alcohol **E103**
 pseudopinene **P198**
 pseudoxanthine **X2**
 psoralen **P344**
 PTBT **B278**
 pteridoxamine **P345**
 pterin **P345**
 Pterofen **T203**
 pteroyl-L-glutamic acid **F96**
 PTFE **P232**
 PTU **P136**
 PTU **P337**
 Pulsar **C34**
 Puma **F16**
 Punch **F90**
 Purasolv **E141**
 purified siliceous earth **D97**
 1*H*-purin-6-amine, *N*-(2-furanylmethyl) **K11**
 purine **P346**
 1*H*-purine **P346**
 7*H*-purine **P346**
 9*H*-purine **P346**

β -purine **P346**
 purine-2,6-diol **X2**
 9H-purine-2,6-diol **X2**
 purine-2,6-1H,3H-dione **X2**
 2,6(1,3)-purinedione **X2**
 purine-6-thiol **M63**
 6-purinethiol **M63**
 Purinethol **M63**
 Purodigin **D335**
 Purpurid **D335**
 Pursuit **I7**
 putrescine **B201**
 Puvalen **M129**
 Puvamet **M129**
 PVA **P234**
 PVAE **P233**
 PVC **P235**
 P.V.P. **P236**
 PX-111 **D578**
 PX-120 **D355**
 PX-126 **D577**
 PX-138 **D519**
 PX-917 **T361**
 pybuthrin **P204**
 Pydrin **F28**
 Pylen **P224**
 pyraclofos **P347**
 Pyrafat **P348**
 Pyramin **C131**
 pyranaldehyde **A36**
 2H-pyrancarboxaldehyde, 3,4-dihydro- **A36**
 pyrathin **M117**
 pyrazinamide **P348**
 pyrazinecarboxamide **P348**
 pyrazine hexahydrate **P200**
 pyrazinoic acid amide **P348**
 pyrazole **P349**
 1H-pyrazole **P349**
 1H-pyrazolo[3,4-d]pyrimidin-4-ol **A70**
 3H-pyrazol-3-one, 4-amino-1,2-dihydro-1,5-dimethyl-2-phenyl- **A113**
 Pyrazone **C131**
 pyrazophos **P350**
 pyrene **P351**
 β -pyrene **P351**
 Pyrenone **P354**
 Pyrethrin **R4**
 Pyrethrin **C344**
 Pyrethrin **C345**
 pyrethrin I **P352**
 pyrethrin II **P353**
 pyrethrins **P354**
 (+)-pyrethrone (+)-pyrethrate **P353**
 pyrethrum **P354**
 pyridaphenthion **P355**
 pyridate **P356**
 2-pyridinamine **A151**
 3-pyridinamine **A152**
 4-pyridinamine **A153**
 α -pyridinamine **A151**
 pyridine **P357**
 2-pyridinecarbonitrile **C487**
 3-pyridinecarbonitrile **C488**
 4-pyridinecarbonitrile **C489**
 3-pyridinecarboxamide **N53**
 β -pyridinecarboxamide **N53**
 pyridine- β -carboxylic acid **N57**
 3-pyridinecarboxylic acid **N57**
 4-pyridinecarboxylic acid hydrazide **I109**
 4-pyridinecarboxylic acid, 2-(1-methylethyl)hydrazide, phosphate **I63**
 4-pyridinecarboxylic acid, 2-[3-oxo-3-[(phenylmethyl)-amino]propyl]hydrazide **N43**
 pyridine, 2-chloro- **C279**
 pyridine, 3-chloro- **C280**
 2,6-pyridinedicarboxylic acid, 4-[2-[2-carboxy-5-(β -D-glucopyranosyloxy)-2,3-dihydro-6-hydroxy-1H-indol-1-yl]ethenyl]-2,3-dihydro-, [5-(R,R)]- **B107**
 pyridine, 2,4-dimethyl- **L62**
 pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-, [R-(R*,R'')]-2,3-dihydroxybutanedioate (2:1) **N56**
 pyridinium, 1-hexadecyl-, chloride **C104**
 α -[(2-pyridinylamino)methyl]benzenemethanol **P140**
 pyridium **P63**
 1H-pyrido[2,3-b]indole **C70**
 5H-pyrido[4,3-b]indole **C72**
 9H-pyrido[2,3-b]indole **C70**
 9H-pyrido[3,4-b]indole **C71**
 1H-pyrido[2,3-b]indole-2-amine **A1**
 pyridoxal hydrochloride **P359**
 pyridoxine **P358**
 pyridoxine hydrochloride **P359**
 pyridoxol **P358**
 4-(pyridyl-2-amidosulfonyl)-3'-carboxy-4'-hydroxyazo-benzene **S140**
 3-pyridylamine **A152**
 4-pyridylamine **A153**
 α -pyridylamine **A151**
 α -[(2-pyridylamino)methyl]benzyl alcohol **P140**
 2-pyridylmethyl chloride hydrochloride **P186**
 N-(3-pyridylmethyl)-N'-(p-nitrophenyl)urea **P362**
 5-[4-(2-pyridylsulfonyl)phenylazo]-2-hydroxybenzoic acid **S140**
 5-[p-(2-pyridylsulfonyl)phenylazo]salicylic acid **S140**
 pyrifeno **P360**
 pyrimethamine **P361**
 2,4-pyrimidinediol **U8**
 2,4(1H,3H)-pyrimidinedione **U8**
 2,4-1H,3H-pyrimidinedione, 5-bis(2-chloroethylamino) **B119**
 2,4,6-(1H,3H,5H)-pyrimidinetrione, 5-butyl-5-methyl **B222**
 N'-2-pyrimidinylsulfanilamide **S132**
 4(1H)-pyrimidone, 5-butyl-2-(ethylamino)-6-methyl- **E70**

pyriminil **P362**
 Pyrimor **P208**
 Pyrimamine **T334**
 pyrinistol **M117**
 pyrinuron **P362**
 pyrithione zinc **Z15**
 pyro **S88**
 pyroacetic ether **A17**
 pyrobenzol **B47**
 pyrobenzole **B47**
 pyrocatechol **C95**
 pyrocatechol dimethyl ether **V18**
 Pyrodust **T68**
 Pyrofax **L59**
 pyrogallic acid **P363**
 pyrogallol **P363**
 pyromellitic dianhydride **P364**
 pyromucic aldehyde **F120**
 pyropentylene **C528**
 pyrophosphate **S88**
 pyrophosphoric acid, tetraethyl ester **T68**
 pyroquilon **P365**
 pyroracemic acid **P368**
 pyrosulfuric acid **S153**
 pyroxylic spirit **M116**
 pyrrodiazole **T204**
 pyrrole **P366**
 1*H*-pyrrole **P366**
 pyrrolidine **P367**
 2-pyrrolidinecarboxylic acid **P284**
 1-[4-(1-pyrrolidinyl)-2-butyryl]-2-pyrrolidinone **O51**
 1*H*-pyrrolo[2,1-*i*][1,4,7,10,13]oxatetraazacyclohexadecine,
 cyclic peptide deriv. **A45**
 1*H*-pyrrolo[2,1-*i*][1,4,7,10,13]oxatetraazacyclohexadecine,
 cyclic peptide deriv. **A46**
 pyrrolylene **B197**
 pyruvic acid **P368**
 QCB **P27**
 QO Fa-Rok **F127**
 Quaalude **M119**
 Quantril **B62**
 quartz **S29**
 quartz **Q1**
 α -quartz **Q1**
 β -quartz **Q1**
 Quaternario LPC **L10**
 Quaternium 13 **M364**
 Quatrac CTAC **C105**
 Quebrachine **Y1**
 Queletox **F24**
 quercetin **Q2**
 quercetin 3-rutinoside **R22**
 Querton 16CI-29 **C105**
 Queschlor **T250**
 Questran (as the chloride) **C325**
 quicklime **C37**
 Quickset extra **M222**
 quicksilver **M64**
 Quiescin **R3**
 Quilan **B29**
 quinacrine **M55**
 quinalbarbitone **Q3**
 quinaldine **Q4**
 quinalphos **Q5**
 quinine **Q6**
 quinizarin **Q7**
 quinochloramine **Q8**
 quinol **H107**
 Quinolin **Q9**
 quinoline **Q9**
 β -quinoline **I135**
 Quinoline Yellow **Q10**
 Quinoline Yellow A **C427**
 Quinoline Yellow Base **C427**
 Quinoline Yellow KT **Q10**
 Quinoline Yellow Spirit Soluble **C427**
 2-quinolinol **H118**
 8-quinolinol **H119**
 8-quinolinol sulfate **H120**
 2(1*H*)-quinolone **H118**
 quinomethionate **Q11**
 quinone **B74**
p-quinone dioxime **B75**
 quinone monoxime **N170**
 quinone oxime **N170**
 Quinophenol **H119**
 Quinothionate **T142**
 Quintox **C323**
 quintozene **Q12**
 quizalofop-ethyl **Q13**
 Quodrole **M210**
 R-152450 **F93**
 R-1607 **V19**
 R-40244 **F87**
 R 113 **T269**
 R 116 **H46**
 R 12 **D204**
 R 161 **F64**
 R 2061 **P17**
 R 21 **D216**
 R 2170 **O57**
 R 218 **O7**
 R 22 **C192**
 R 23 **T292**
 R 23979 **I4**
 R 25788 **D171**
 R 31 **C200**
 Rabcide **P174**
 Rabon **T60**
 Raboral **O62**
 racemic tartaric acid **T8**
 racer **F87**
 Racumin D **C323**
 Radeks **C480**

Radiant Red Lake **C418**
 Radiaquat 6444 **C105**
 radon **R1**
 Radosan **M137**
 Ragadan **H29**
 Rally **M360**
 Ralox BHT food grade **B245**
 Ramik **D535**
 Rampage **C323**
 Randal **F18**
 Randox **A69**
 raney copper **C429**
 Rangado **D460**
 Ranger **D368**
 Ratak **B150**
 Raticate **N201**
 Ratilan **C445**
 RATO **T224**
 Ratofin **F116**
 Ratol **Z14**
 Rat-a-Way **F116**
 raunormine **D58**
 Rausedyl **R3**
 RC-318 **O5**
 RCRA waste number P013 **B12**
 RCRA waste number P030 **C481**
 RCRA waste number P054 **A266**
 RCRA waste number P056 **F52**
 RCRA waste number P060 **I101**
 RCRA waste number P121 **Z8**
 RCRA waste number U042 **C199**
 RCRA waste number U052 **C456**
 RCRA waste number U052 **C459**
 RCRA waste number U052 **C457**
 RCRA waste number U052 **C458**
 RCRA waste number U055 **C474**
 RCRA waste number U151 **M64**
 RD 1572 **E65**
 RDX **R2**
 Readex **T142**
 recanescine **D58**
 Recif **H43**
 Recozit Wuehlmaus-Gas **C24**
 Rectobania **O40**
 Redax **N155**
 red copper oxide **C440**
 Red Hot Pellets **C33**
 Redisol **C368**
 red mercuric iodide **M76**
 red oxide of mercury **M82**
 Red RL Base **M259**
 Reducor **P321**
 Reducymol **A207**
 Reevon **P224**
 Reflex **F98**
 Refurthiozole **N59**
 Regazol **D560**

Regent **F33**
 Regesan **D260**
 Reglex **D561**
 Reglone **D561**
 Regulox **M14**
 Regutol **D583**
 Relact **N67**
 Reldan **C314**
 Remanex **T63**
 Renafur **N58**
 Renegade **C543**
 Repellent 1207 **C277**
 Reply **C480**
 resbenzophenone **B85**
 Resectisol **M28**
 reserpidine **D58**
 reserpine **R3**
 resin acids and rosin acids, aluminium salts **A106**
 resin acids and rosin acids, cobalt salts **C377**
 Resinase **L51**
 Resisan **D260**
 Resistamine **T334**
 resmethrin **R4**
 resorcin **R5**
 resorcinol **R5**
 resorcinol diglycidyl ether **R6**
 resorcinolphthalein **F51**
 resorcinol phthalein sodium **C399**
 Respenyl **G47**
 Restamine **D537**
 Restinyl **M117**
 Retarder AK **P173**
 Retarder BA **B63**
 Retarder BAX **B63**
 Retarder ESEN **P173**
 Retarder PD **P173**
 Retardo **P74**
 13-*cis*-retinoic acid **I138**
 retinol **R7**
 retinol (all-*trans*) **R7**
 Reumuzol **P96**
 Revonal **M119**
 Reward **V19**
 Rezifilm **T147**
 RH-893 **O19**
 RH 2915 **O59**
 RH 315 **P339**
 RH 787 **P362**
 rhabarberone **A95**
 RH 2915D **O59**
 rheinzink **Z2**
 rhenium **R8**
 Rhenogram SF ETU-50 **E122**
 Rhenogran DETU-80 **D318**
 Rhenogran DPG-80 **D545**
 Rhenogran TDEC-75 **E174**
 Rhenogran TETD-75 **D565**

Rhenomag **M6**
 Rhizopin **I32**
 Rhodacide **E68**
 rhodamine B **R9**
 rhodamine 6G **C401**
 Rhodapos **P233**
 rhodeose **F114**
 Rhodialothen **H4**
 Rhodiatox **P13**
 rhodium **R10**
 rhodium(III) chloride **R11**
 rhodium chloride (RhCl₃) **R11**
 rhodium trichloride **R11**
 Rhoduline Orange **C421**
 Ribipca **R12**
 Riboderm **R12**
 riboflavin **R12**
 riboflavine **R12**
 1-β-D-ribofuranosyluracil **U15**
 rice starch **S110**
 Ricid II **I61**
 ricin **R13**
 Ricine **R13**
 Ricins **R13**
 Ricketon **C323**
 Ridall **Z14**
 riddelliin **R14**
 riddelliine **R14**
 Ridect **T60**
 ridelline **R14**
 Ridomil **M93**
 rifa **R15**
 rifadin **R15**
 rifampicin **R15**
 rifampin **R15**
 riforal **R15**
 Rilof **P205**
 Rimidin **F4**
 Rimidine **F4**
 Riprin **E16**
 Ritatin **B112**
 Rivadorm **P45**
 Ro 10-9359 **E184**
 Ro 7-6145 **D362**
 road tar **A249**
 Roan **T226**
 Robimycin **E47**
 Robitussin **G47**
 Roccal **A66**
 Rodafarin **W1**
 Rodent Cake **D535**
 Rodentin **C448**
 Rodex **F53**
 Rodocid **E68**
 Rody **F18**
 Rogodial **P89**
 Rokar X L **B151**

Roksol T1-7 **H51**
 Romicil **O29**
 Ro-Neet **C498**
 Ronilan **V23**
 Ronnel **F8**
 Ronstar **O44**
 Ro-Papav **P5**
 Rosaniline **M1**
p-rosaniline HCl **C402**
 Rose Bengal sodium **R16**
 Rosemide **F112**
 rosin oil **R17**
 Rospan **C276**
 Rospin **C276**
 Rotacide **R18**
 Rotate **B28**
 rotax **M61**
 rotenone **R18**
 Rovimix A 500 **V40**
 Rovral **I62**
 Roxanthin Red 10 **C413**
 Rozol **C238**
 Roztoczol **T63**
 RP 13057 **D23**
 RP 17623 **O44**
 RP 23669 **I12**
 RP 9895 **V9**
 RPA 41670H **D327**
 RS Nitrocellulose **C98**
 RU22974 **D46**
 Ruban **B37**
 rubene **N6**
 Ruberon **P116**
 Ruberon granule **E144**
 rubidium **R19**
 rubidium hydroxide **R20**
 rubidium hydroxide (RbOH) **R20**
 rubidomycin **D23**
 Rubidor **A259**
 Rubigan **F4**
 rubimycin C **D23**
 Rubine Toner 2BS **C418**
 Rubitox **P149**
 Ruelene **C471**
 Rugby **C15**
 Rulene **C471**
 Rustol-HED **T217**
 ruthenium **R21**
 rutin **R22**
 rutoside **R22**
 Ryzelan **O36**
 S-1046 **X16**
 S-47 **B166**
 S-6999 **N201**
 Sabel **E72**
 saccharin **S1**
 saccharose **S131**

SADH **D21**
 Safidon **P153**
 Safranin B Extra **P82**
 safrole **S2**
 Safrotin **P304**
 Sag **T194**
 Salamid **S5**
 Salazopyrin **S140**
 salazosulfapyridine **S140**
 Salbulin Inhaler **S3**
 salbutamol **S3**
 salenixum **P253**
 sal ethyl **E169**
 Salicylal **S4**
 salicylaldehyde **S4**
 salicylamide **S5**
 salicylazosulfapyridine **S140**
 salicylic acid **S6**
 salicylic acid acetate **A28**
 salicylic acid, choline salt **C327**
 salicylic acid, (hydromercuri)-, cyclic anhydride **M84**
 salicylic acid, phenyl ester **P132**
 salicylic acid with physostigmine (1:1) **P179**
 salicylic aldehyde **S4**
 salicylic ether **E169**
 salipuro **N31**
 salipurpol **N31**
 Salithion **D527**
 Salix **F112**
 salol **P132**
 Salphenyl **P132**
 sal polychrestum **P264**
 Salt cake **S92**
 salt of saturn **L12**
 saltpeter **P257**
 Saluric **C287**
 sal volatile **A168**
 samarium **S7**
 SAN 197 **E186**
 Sanamycin **A45**
 Sanatir **F26**
 sand **Q1**
 Sandafan **O45**
 Sandocryl Blue BRL **M216**
 SAN 371F **O45**
 Sanger's reagent **D476**
 Sanimul **E74**
 Saniticer 160 **B94**
 Sanspor **C58**
 Santar SM **C58**
 Santhane **C59**
 Santoflex **E85**
 Santoquin **E85**
 Santotherm **A239**
 Santowax M **T29**
 Santowax P **T31**
 Sanyo Fast Red B Base **M141**
 Saphicol **M50**
 Saphizon **M50**
 Sapilent **T328**
 Sappiran **C127**
 Sapro **T295**
 DL-sarcosine **M88**
 L-sarcosine **M49**
 sarin **S8**
 Sarlate **P230**
 Sarodormin **G22**
 Satintone **K2**
 Satisfar **E186**
 Satocide **P80**
 Saverit **V19**
 Savirox **V19**
 Sayfos **M50**
 SB 1528 **P54**
 SBa 0108E **B11**
 Scam **E85**
 Scarlet G Base **M260**
 Scav-Ox **H87**
 α-Schardinger dextrin **C500**
 β-Schardinger dextrin **C501**
 γ-Schardinger dextrin **C502**
 Schercemol DIA **D357**
 Schering 36103 **F106**
 schradan **S9**
 Schultz no.958 **P82**
 scilliroside **S10**
 Scintillar **X7**
 scopolamine **H122**
 scopolamine bromide **H123**
 Scorpio **D368**
 Scout **T194**
 SDMH **D421**
 SDS **S76**
 Seagel L **L57**
 Sea Kem **C91**
 sebacic acid **S11**
 Sebacyl **P170**
 secobarbital **Q3**
 (3β,5Z,7E)-9,10-secocholesta-5,7,10(19)-trien-3-ol **C323**
 9, 10-secocholesta-5,7,10(19)-trien-3β-ol **C323**
 (3β,5Z,7E,22E)-9,10-secoergosta-5,7,10(19),22-tetraen-3-ol **E42**
 seconal **Q3**
 Securex **T128**
 Sedopretten **D538**
 Sefsol 810 **T224**
 Seftal **C59**
 selane **H104**
 Selemide **D536**
 selenic acid **S12**
 selenic acid, disodium salt **S89**
 seleninyl chloride **S19**
 selenious acid **S13**
 selenious acid, disodium salt **S90**

selenious anhydride **S16**
 selenium **S14**
 selenium diethyldithiocarbamate **S15**
 selenium dioxide **S16**
 selenium(IV) dioxide **S16**
 selenium disulfide **S17**
 selenium fluoride (SeF₆) **S18**
 selenium hexafluoride **S18**
 selenium hydride **H104**
 selenium monosulfide **S20**
 selenium oxide **S16**
 selenium oxychloride **S19**
 selenium sulfide **S20**
 selenium sulfide (SeS₂) **S17**
 selenium tetrakis(diethyldithiocarbamate) **S15**
 selenourea **S21**
 2-selenourea **S21**
 selenouronium **S21**
 selenous acid **S13**
 Selsun blue **S17**
 Semeron **D60**
 Semevin **T128**
 semicarbazine hydrochloride **S22**
 semicarbazine monohydrochloride **S22**
 semidine **P128**
 Semikon **M117**
 Semikon hydrochloride **M118**
 seminose **M30**
 Sendoxan **C529**
 senecionan-11,16-dione, 13,19-dihydro-12,18-dihydroxy-
R14
 senfgas **M359**
 senkirkine **S23**
 Sentry Dimethicone **D373**
 Sepsinol **F122**
 Sequestrene **E8**
 Sequestrene Na₂Ca **E4**
 Sequestrene trisodium **E9**
 Seradix **I34**
 DL-serine **S24**
 1-serine diazoacetate **A260**
 serpentine **C342**
 serpentine chrysotile **C342**
 Serpine **R3**
 Setacyl Diazo Navy R **D95**
 sethoxydim **S25**
 sevin **C63**
 Sextol **M198**
 Sextol **M201**
 Sexton B **M203**
 Sextone B **M197**
 Shellsol-140 **N193**
 Sheriff **C83**
 Shield **C364**
 shikimic acid **S26**
 Shoxin **N201**
 Sicid **R18**

Siclor **C286**
 Sico Red WRC **C418**
 siduron **S27**
 silane **S28**
 silane, (4-aminobutyl)diethoxymethyl- **A122**
 silane, chlorotrihexyl- **C303**
 silane, chlorotrimethyl- **C304**
 silane, chlorotriphenyl- **C305**
 silane, 3-cyclohexenyltrichloro- **C512**
 silane, diethoxydimethyl-, **D284**
 silane, trichloro-2-propenyl- **A94**
 Silasorb **C43**
 silica **S29**
 silica, crystalline **Q1**
 silica gel **S29**
 silica glass **S29**
 silicane **S28**
 silicate(2-), hexafluoro-, diammonium **A174**
 silicate(2-), hexafluoro-, disodium **S68**
 silicate(2-), hexafluoro-, lead(2+)(1:1) **L23**
 silicic acid, calcium salt **C43**
 silicic acid, tetramethyl ester **T91**
 silicic anhydride **Q1**
 silicochloroform **T267**
 silicofluoric acid **F74**
 silicofluoride **F73**
 silicon **S30**
 silicon carbide **S31**
 silicon chloride hydride **T267**
 silicone 360 **S32**
 silicone, di-Me **S32**
 silicone oil **S32**
 silicon ethoxide **T67**
 silicon fluoride magnesium salt **M4**
 silicon hexafluoride ion **F73**
 silicon methoxide **T91**
 silicon monocarbide **S31**
 silicon sodium fluoride **S68**
 silicon tetraethoxide **T67**
 silicon tetrahydride **S28**
 Silikan L **T67**
 siloxane **S32**
 Siltex gum **K3**
 Silutin **D315**
 Silvan **M228**
 silver **S33**
 silver arsenite **S34**
 silver cyanide **S35**
 silver matt powder **T158**
 silver nitrate **S36**
 silver potassium cyanide **P262**
 Silvex **F14**
 simazine **S37**
 simetryn **S38**
 Simidan **P153**
 Simplene **A51**
 Sinbor **T20**

Sinerdol **R15**
 Sinomin **S136**
 Sinotol **G47**
 Sinovula **N207**
 Sintas 90 **F104**
 Sionite **S104**
 Siosan **S104**
 Sipon LS **S76**
 size precipitate **A106**
 Skane M-8 **O19**
 Skellysolve A **P39**
 Skipper **T128**
 slaked lime **C33**
 Slam C **A273**
 Slimetrol RX-39 **B182**
 SLJ-312 **F40**
 Sloggy **T128**
 Slopvox **P7**
 SMA **S55**
 Smash **F18**
 Smite **S47**
 Smite **C314**
 Smoke Orange R **Q7**
 SN 38584 **P78**
 Snip **A259**
 Snowflake 30091 **S110**
 Snowit **Q1**
 Soapstone **T3**
 sobitat-K **P263**
 Sobrol A **E158**
 soda **S52**
 soda ash **S52**
 soda ash flux-calcined Kieselguhr **D97**
 soda lye **S73**
 sodamide **S41**
 soda niter **S80**
 sodium **S39**
 sodium acetate **S40**
 sodium acid sulfite **S48**
 sodium aluminium fluoride **C472**
 sodium amide **S41**
 sodium-*p*-aminobenzenearsonate **S43**
 sodium aminophenol arsonate **S43**
 sodium-*p*-aminophenylarsonate **S43**
 sodium anilarsonate **S43**
 sodium anthraquinone-1-sulfonate **S42**
 sodium arsanilate **S43**
 sodium arsenate **S44**
 sodium *o*-arsenate **S44**
 sodium arsenic oxide **S45**
 sodium arsenite **S45**
 sodium ascorbate **S46**
 sodium azide **S47**
 sodium baborate **B141**
 sodium bifluoride **S71**
 sodium bisulfide **S72**
 sodium bisulfite **S48**
 sodium bithionolate **S49**
 sodium borate decahydrate **B141**
 sodium borohydride **S50**
 sodium bromate **S51**
 sodium bromeborate **C547**
 sodium cacodylate **S63**
 sodium calcium edetate **E4**
 sodium carbolate **S85**
 sodium carbonate **S52**
 sodium chlorate **S53**
 sodium chlorite **S54**
 sodium chloroacetate **S55**
 sodium chromate **S56**
 sodium chromate(VI) **S56**
 sodium chromoglycate **S57**
 sodium cumeneazo- β -naphthol disulfonate **C414**
 sodium cyanide **S58**
 sodium cyclamate **S59**
 sodium cyclohexylsulfamate **S59**
 sodium dehydroacetate **S60**
 sodium 2,2-dichloropropionate **D20**
 sodium dichromate **S61**
 sodium dichromate dihydrate **S62**
 sodium diethylaminocarbodithioate **D575**
 sodium diethyldithiocarbamate **D575**
 sodium 4-dimethylaminobenzenediazosulfonate **F2**
 sodium *p*-(dimethylamino)benzenediazosulfonate **F2**
 sodium dimethylaminocarbodithioate **S64**
 sodium 4-[(4-dimethylamino)phenylazo]benzenesulfonate **M271**
 sodium dimethylarsinate **S63**
 sodium dimethylarsonate **S63**
 sodium dimethyldithiocarbamate **S64**
 sodium 2,4-dinitrophenate **D490**
 sodium 2,4-dinitrophenol **D490**
 sodium 2,4-dinitrophenolate **D490**
 sodium 5,5-diphenylhydantoinate **P142**
 sodium 5,5-diphenyl-2,4-imidazolidinedione **P142**
 sodium dipropylacetate **S100**
 sodium ditolyldiazobis-8-amino-1-naphthol-3,6-disulfonate **T366**
 sodium DNP **D490**
 sodium dodecylbenzenesulfonate **S65**
 sodium dodecyl sulfate **S76**
 sodium edetate **E8**
 Sodium eosin **E29**
 sodium ethanoate **S40**
 sodium ethidronate **D562**
 sodium fluoresceinate **C399**
 sodium fluoride **S66**
 sodium fluoroacetate **S67**
 sodium fluorophosphate **D563**
 sodium fluorosilicate **S68**
 sodium *E,E*-2,4-hexadienoate **S91**
 sodium hexafluoroaluminate **C472**
 sodium hexametaphosphate **S69**
 sodium hydrate **S73**

sodium hydride **S70**
 sodium hydroborate **S50**
 sodium hydrogen difluoride **S71**
 sodium hydrogen fluoride **S71**
 sodium hydrogen methylarsenate **M355**
 sodium hydrogen sulfide **S72**
 sodium hydrogen sulfite **S48**
 sodium hydrosulfide **S72**
 sodium hydroxide **S73**
 sodium hypochlorite **S74**
 sodium hypochlorite pentahydrate **S75**
 sodium isopropylxanthate **P343**
 sodium laurylbenzenesulfonate **S65**
 sodium lauryl sulfate **S76**
 sodium mercaptan **S72**
 sodium mercurhydrin **S77**
 sodium metaarsenite **S45**
 sodium metabisulfite **S78**
 sodium methylarsenate **D601**
 sodium methyldithiocarbamate **M96**
 sodium monochloroacetate **S55**
 sodium monofluoride **S66**
 sodium monofluoroacetate **S67**
 sodium monofluorophosphate **D563**
 sodium monohydride **S70**
 sodium monohydrogen phosphate **S79**
 sodium monosulfide **S93**
 sodium nitrate **S80**
 sodium nitrite **S81**
 sodium pentachlorophenol **S82**
 sodium pentachlorophenolate **S82**
 sodium pentachlorophenoxide **S82**
 sodium perchlorate **S83**
 sodium peroxydisulfate **S84**
 sodium persulfate **S84**
 sodium phenate **S85**
 sodium phenolate **S85**
 sodium phenoxide **S85**
 sodium *o*-phenylphenate **S86**
 sodium *o*-phenylphenolate **S86**
 sodium *o*-phenylphenoxide **S86**
 sodium phenytoin **P142**
 sodium phosphate, dibasic **S79**
 sodium phosphate dodecahydrate **T360**
 sodium phosphate ($\text{Na}_5\text{P}_3\text{O}_{10}$) **S98**
 sodium phosphate ($\text{Na}_6\text{P}_6\text{O}_{18}$) **S69**
 sodium phosphate, tribasic **T359**
 sodium phosphide **S87**
 sodium 2-propylpentanoate **S100**
 sodium pyroborate **B141**
 sodium pyrophosphate **S88**
 sodium pyrosulfite **S78**
 sodium selenate **S89**
 sodium selenite **S90**
 sodium selenium oxide **S90**
 sodium silicon fluoride **S68**
 sodium sorbate **S91**
 sodium sulfate **S92**
 sodium sulfate (anhydrous) **S92**
 sodium sulfhydrate **S72**
 sodium sulfide **S93**
 sodium sulfite **S94**
 sodium tellurite **S95**
 sodium tellurite(IV) **S95**
 sodium tellurium oxide **S95**
 sodium tetraborate **B141**
 sodium tetraborate **S96**
 sodium 2,2,3,3-tetrafluoropropanoate **F83**
 sodium 2,2,3,3-tetrafluoropropionate **F83**
 sodium tetrahydridoborate **S50**
 sodium tetrahydroborate **S50**
 sodium *p*-toluenesulfonylchloramide **C113**
 sodium trichloroacetate **S97**
 sodium triphosphate **S98**
 sodium tripolyphosphate **S98**
 sodium tungstate **S99**
 sodium tungstate(VI) **S99**
 sodium valproate **S100**
 sodophos **M11**
 Soilsin **E144**
 Solactol **E141**
 Solatene **C89**
 Solethion **E68**
 Solgard **P209**
 Solicam **N206**
 solid crotonic acid **C468**
 Soliviol **E76**
 solketal **S101**
 solubacter **T270**
 soluble phenytoin **P142**
 Solvent 111 **T247**
 Solvent M **M147**
 Solvent Red 43 **E29**
 Solvent Yellow 33 **C427**
 Solvirex **D566**
 Solvor **P234**
 Sombulex **H76**
 Sominat **D170**
 Somnalert **H76**
 Somnos **C108**
 Somonal **P79**
 Sonac **P156**
 Sonacide **G21**
 Sonalan **E56**
 Sonalen **E56**
 Sonapax **T143**
 Sonar **F86**
 Sonebon **N67**
 soprocide **H9**
 Sorbex **S104**
 sorbic acid **S102**
trans,trans-sorbic acid **S102**
 sorbic acid, potassium salt **P263**
 sorbic acid, sodium salt **S91**

sorbic oil **P12**
 sorbimacrogol laurate **P227**
 Sorbistat **S102**
 sorbitan, monododecanoate **S103**
 sorbitan monolaurate **S103**
 sorbitan polyethoxy monostearate **P229**
 D-sorbitol **S104**
 Sorbol **S104**
 Sorexal **E42**
 Sorgen 90 **S103**
 Sorilan **F19**
 Sosigon **P42**
 SP230 **N12**
 Span 20 **S103**
 Sparine **P285**
 Sparkstar **D372**
 sparteine **S105**
 Sparticide **F67**
 Special Pitch 4 **C366**
 spectracide **D99**
 spermidine **S106**
 spermine **S107**
 Spica 300 **P182**
 Spidoxol **P117**
 Spike **T13**
 spinacene **S109**
 Spinnaker **T197**
 spirit of ethyl nitrite **E156**
 spirits of turpentine **T374**
 spiro[17*H*-cyclopento[*a*]phenanthrene-17,2'(5'*H*)furan],
 pregn-4-ene-21-carboxylic acid derivative **S108**
 Spirofulrin **G46**
 spironolactone **S108**
 Spirosal **G38**
 Spotton **F24**
 Sprayset MEKP **M222**
 Spur **F94**
 squalene **S109**
E,E,E,E-squalene **S109**
trans-squalene **S109**
 SR-379 **G31**
 SR 1354 **M335**
 SSH **I139**
 Staa-Free **B151**
 Stabilizer 2013-P **C479**
 Stabinex NC₁₈ **L20**
 Stamere **C91**
 Stannane, acetyloxytriphenyl- **F25**
 stannane, chlorotriphenyl **T340**
 stannane, trichlorooctyl- **O24**
 stannane, tricyclohexylhydroxy- **C535**
 stannic chloride **T160**
 stannic tetrachloride **T160**
 stannous dichloride **T159**
 stannous fluoride **T161**
 Stanycin **N210**
 Stanzamine **T334**
 Starane **F88**
 starch **S110**
 Stauroderm **F84**
 Stazepin **C61**
 stearamine **S111**
 Stearex Beads **S112**
 stearic acid **S112**
 stearic acid, cadmium salt **C12**
 stearic acid, zinc salt **Z16**
 stearophanic acid **S112**
 stearyl alcohol **S113**
 stearylamine **S111**
 Steatite **T3**
 Steclin **T62**
 stenol **S113**
 Stepanol WAC **S76**
 Sterane **P269**
 Sterazine **S132**
 sterigmatocystin **S114**
 Sterisil **H75**
 stibine, trichloro- **A225**
 stibine, trifluoro- **A226**
 stilbene **S115**
 4,4'-stilbenediol, α,α' -diethyl-, dipropionate, (*E*)- **S117**
 stilbestrol **S116**
 stilbestrol dipropionate **S117**
 stilbestrol monoglucuronide **S118**
 Stinerval **P64**
 Stinger **C364**
 stink damp **H105**
 Stirpan **D512**
 Stock Guard **F43**
 Stoddard solvent **S119**
 Stomp **P20**
 Stopper **H80**
 Storm **F37**
 STRZ **S120**
 Stratagem **F37**
 streptozocin **S120**
 streptozotocin **S120**
 strobane **P221**
 Strodival **O40**
 strontium **S121**
 strontium chromate **S122**
 strontium dinitrate **S123**
 strontium nitrate **S123**
 strontium phosphide **S124**
 strontium yellow **S122**
 K-strophanthin- α **C536**
 Strophoperm **O40**
 strychnidin-10-one **S125**
 strychnin **S125**
 strychnine **S125**
 styrallyl alcohol **P68**
 styrene **S126**
 styrene oxide **S127**
 styrene polymer **P231**

styrofoam **P231**
 styrol **S126**
 styrolene **S126**
 styron **P231**
 styryl oxide **S127**
 Su 13437 **N2**
 subchloride of mercury **M70**
 Subdue **M93**
 sucaryl **C495**
 sucaryl acid **C495**
 Sucaryl Sodium **S59**
 succinic acid **S128**
 succinic acid dinitrile **S130**
 succinic acid, mercapto-, diethyl ester, *S*-ester with *O,O*-dimethyl phosphorothioate **M10**
 succinic acid, mono(2,2-dimethylhydrazide) **D21**
 succinic acid peroxide **D564**
 succinic anhydride **S129**
 Succinil **S130**
 succinonitrile **S130**
 (succinyldioxy)bis[tributylstannane] **T221**
 succinyl oxide **S129**
 succinyl peroxide **D564**
 sucinonitrile **S130**
 Sucrol **E81**
 Sucrosa **S59**
 sucrose **S131**
 D-sucrose **S131**
 Sudan I **C426**
 Sudan II **C420**
 Sudan III **C422**
 Sudan Orange **C420**
 Sudan Orange R **C426**
 Sudan Yellow GC **M320**
 Suffix **B84**
 Suffix BW **F35**
 Sufran **S149**
 sugar **S131**
 sugar of lead **L12**
 Sulcatone **M232**
 Sulfabid **S139**
 Sulfacetil **P177**
 Sulfactin **D369**
 sulfadiazine **S132**
 sulfadimidine **S133**
 Sulfafurazole **S141**
 sulfaguanidine **S134**
 Sulfaguine **S134**
 sulfallate **S135**
 sulfamethoxazole **S136**
 sulfamethoxizole **S136**
 sulfamic acid **S137**
 sulfamic acid, cobalt(II) salt (2:1) **C378**
 sulfamic acid, dimethyl-, 5-butyl-2-(ethylamino)-6-methyl-4-pyrimidinyl ester **B193**
 sulfamidic acid **S137**
 sulfamidine **S133**
 Sulfan **S157**
 5-sulfanilamido-1-phenylpyrazole **S139**
 sulfanilic acid **S138**
m-sulfanilic acid **M97**
o-sulfanilic acid **A211**
 sulfaphenazole **S139**
 sulfasalazine **S140**
 sulfate lignin **L42**
 Sulfathalidine **P177**
 Sulfazin **S132**
 sulferrous **I76**
 sulfethylic acid **E173**
 Sulfidophos **F24**
 1,1'-sulfinylbisbenzene **P135**
 sulfinylbis(methane) **D458**
 sulfenyl chloride **T136**
 sulfisomezole **S136**
 sulfisoxazole **S141**
 sulfluramid **S142**
 sulfobenzide **P134**
o-sulfobenzimide **S1**
o-sulfobenzoic acid imide **S1**
 sulfocarbonilide **T123**
 sulfocarbonic anhydride **C75**
 Sulfoguanyl **S134**
 sulfolane **S143**
 3-sulfolene **S144**
 β-sulfolene **S144**
 sulfometuron-methyl **S145**
 1-(4-sulfo-1-naphthylazo)-2-naphthol-3,6-disulfonic acid, trisodium salt **A108**
 Sulfonax **D589**
 1,1'-sulfonylbisbenzene **P134**
 4,4'-sulfonylbisbenzeneamine **S146**
 1,1'-sulfonylbis(4-chlorobenzene) **B127**
 1,1'-sulfonylbisethene **V38**
 sulfonylbismethane **D457**
 4,4'-sulfonyldianiline **S146**
 3-(sulfonyl)-*O*-((methylamino)carbonyl)oxime-2-butanone **B225**
 Sulfopon WA2 **S76**
 sulfotep **S147**
 sulfovinic acid **E173**
 sulfoxide **S148**
 Sulfoxol **S141**
 sulfoxyl **S148**
 Sulframin 85 **S65**
 sulframin acid 1298 **D589**
 sulfur **S149**
 sulfurated hydrogen **H105**
 sulfurated lime **C46**
 sulfur chloride oxide **T136**
 sulfur dioxide **S150**
 sulfur dioxide solution **S155**
 sulfur fluoride (S₂F₁₀) **D568**
 sulfur fluoride (SF₆) **S151**
 sulfur hexafluoride **S151**

sulfur hydride **H105**
 sulfuric acid **S152**
 sulfuric acid, aluminium potassium salt **A105**
 sulfuric acid, ammonium iron (2+) salt **I67**
 sulfuric acid, ammonium nickel(2+) salt (2:2:1) **N45**
 sulfuric acid, barium salt (1:1) **B24**
 sulfuric acid, beryllium salt **B106**
 sulfuric acid, cadmium salt **C13**
 sulfuric acid, calcium salt (1:1) **C44**
 sulfuric acid, calcium salt (1:1), dihydrate **C45**
 sulfuric acid, chromium(3+) salt (3:2) **C338**
 sulfuric acid, cobalt(II) salt (1:1) **C379**
 sulfuric acid, copper(2+) salt (1:1) **C442**
 sulfuric acid, copper(II) salt, ammoniated **C443**
 sulfuric acid, diammonium salt **A185**
 sulfuric acid, diethyl ester **D317**
 sulfuric acid, dimercury(1+) salt **M85**
 sulfuric acid, dimethyl ester **D455**
 sulfuric acid, dipotassium salt **P264**
 sulfuric acid, dithallium(1+) salt **T108**
 sulfuric acid (fuming) **S153**
 sulfuric acid, iron (2+) salt (1:1) **I76**
 sulfuric acid, lead(2+) salt (1:1) **L30**
 sulfuric acid, monododecyl ester, sodium salt **S76**
 sulfuric acid, nickel(2+) salt (1:1) **N50**
 sulfuric acid, thallium salt **T104**
 sulfuric acid, thallium(1+) salt **T108**
 sulfuric acid, zinc salt (1:1) **Z17**
 sulfuric acid, zirconium(IV) salt (2:1) **Z23**
 sulfuric anhydride **S157**
 sulfuric chlorohydrin **C285**
 sulfur monochloride **S154**
 sulfur mustard **M359**
 sulfurous acid **S155**
 sulfurous acid, 2-(*p*-*tert*-butylphenoxy)cyclohexyl 2-propynyl ester **P300**
 sulfurous acid 2-(*p*-*tert*-butylphenoxy)-1-methylethyl 2-chloroethyl ester **A232**
 sulfurous acid 2-chloroethyl 2-[4-(1,1-dimethylethyl)phenoxy]-1-methylethyl ester **A232**
 sulfurous acid, 2-[4-(1,1-dimethylethyl)phenoxy]cyclohexyl 2-propynyl ester **P300**
 sulfurous acid, disodium salt **S94**
 sulfurous acid, monosodium salt **S48**
 sulfurous anhydride **S150**
 sulfurous dichloride **T136**
 sulfurous oxide **S150**
 sulfurous oxychloride **T136**
 sulfur oxychloride **T136**
 sulfur phosphide **P162**
 sulfur selenide **S20**
 sulfur subchloride **S154**
 sulfur superoxide **S150**
 sulfur tetrafluoride **S156**
 sulfur trioxide **S157**
 sulfuryl difluoride **S158**
 sulfuryl fluoride **S158**

Sulgin **S134**
 sulphadiazine **S132**
 sulphadimidine **S133**
 sulphaguanidine **S134**
 Sulphaxalazine **S140**
 sulprofos **S159**
 Sulqui **N52**
 δ -sultone **B210**
 Sumi 8 **D464**
 Sumi-alfa **E49**
 Sumi-alpha **E49**
 Sumicidin **F28**
 Sumicidin A α **E49**
 Sumigard **E49**
 Sumi-gold **E49**
 Sumiherb **B166**
 Sumithrin **P84**
 Summetrin **P3**
 Summit **T197**
 Sumquat 6050 **C103**
 Sunaptic B **N12**
 Sundaram 1975 **P154**
 Sunset Yellow FCF **C415**
 Supasac **S1**
 Supercol **G51**
 Superfanox **D511**
 Super K **P243**
 Supernox **P295**
 Superol **G25**
 Superprednol **D62**
 Supersect **C542**
 Superseptyl **S133**
 Super VMP **N5**
 Suponate DS4 **S65**
 supracyde **M121**
 suprathim **M121**
 Suprex clay **K2**
 Surchlor **S74**
 Surfac CABS70 **C32**
 Surfac CAT176 **C105**
 Surflan **O36**
 Surgex **N43**
 surmontil **T328**
 Susadrin **G26**
 Sustane BHA **B244**
 Sustane 1-F **B244**
 Sustane PG **P332**
 Sutan **B243**
 Sutar **B243**
 Suxil **S130**
 Suzon **C131**
 Swedish Green **P15**
 Sweeta **S1**
 sweet birch oil **M305**
 Swim Clear **C34**
 Syltherm XLT **P222**
 Sylvan **M228**

sylvic acid **A2**
 Sympal **T155**
 Symphonie **F92**
 Symuler fast yellow GF **D96**
 Syncal SDI **S1**
 Synchrovet **O41**
 Syncrolube **P235**
 Syngesterone **P282**
 Synklor **C118**
 Synkrolith **C472**
 Synpro Cadmium Stearate **C12**
 synthetic mustard oil **A87**
 Systhane 6Flo **M360**
 2,4,5-T **T1**
 T60 **T164**
 TA12 **T26**
 Tabamex **B232**
 Tab gum **K3**
 Tabun **T2**
 TAC 121 **T167**
 Tachigaran **H121**
 TACK **C299**
 talc **T3**
 Talcid **H108**
 Talcum **T3**
 Talidene **P177**
 N-tallow-1,3-propanediamine **T4**
 Talodex **F24**
 Talon **B150**
 Talstar **B109**
 Talwin **P42**
 Tamaron **M111**
 Tame **F18**
 Tamex **B232**
 tamoxifen **T5**
 TA-33MP **T26**
 Tanderil **O63**
 Tandex **K4**
 tannic acid **T6**
 tannin **T6**
 tantalum **T7**
 TAP85 **H10**
 Tapazole **M122**
 Tapsin **T137**
 tarapacaite **P244**
 tar camphor **N9**
 Taredan **C15**
 tar oil **C453**
 Tartan **C490**
 tartar emetic **A222**
 DL-tartaric acid **T8**
 L-tartaric acid **T9**
 Tarzol **F5**
 Task **F20**
 Tatevil **T203**
 TB 66 **P217**
 TBA **B241**
 2,3,6-TBA **T10**
 TBBA **T39**
 TBBA **B249**
 TBBPA **T39**
 TBE **T40**
 TBEP **T348**
 T-BGE **B260**
 TBHP **B261**
 TBHQ **B262**
 (T-4)-bis(nitrato-O)dioxouranium **U11**
 TBP **T212**
 TBS **T208**
 TBTO **T219**
 TCA **T226**
 TCA-sodium **S97**
 TCB **T46**
 TCB **T243**
 2,3,6-TCB **T10**
 TCBA **T243**
 2,3,6-TCBA **T10**
 TCC **T270**
 TCDD **D110**
 TCH **T124**
 T-Chlor **S74**
 TCMTB **T125**
 TCNA **T53**
 TCPA **C124**
 TCP (antiseptic) **T258**
 TCP (plasticiser) **T361**
 TDE **D30**
 p,p'-TDE **D30**
 TDI **T175**
 2,4-TDI **T176**
 2,6-TDI **T177**
 TEA **T278**
 teaberry oil **M305**
 Tebrazid **P348**
 tebuconazole **T11**
 tebufenozide **T12**
 tebuthiuron **T13**
 TEC **T279**
 tecnazene **T14**
 TECP **T55**
 Tecquinol **H107**
 Tedion **T63**
 TEDP **S147**
 Teflon **P232**
 tefluthrin **T15**
 TEG **T64**
 Tegafur **F118**
 Tegison **E184**
 Tegosept M **M272**
 Tegratal **C61**
 Tektamer 38 **B163**
 TEL **T66**
 Telar **C315**
 Teldrin **C308**

telepathine **H7**
 Telesmin **C61**
 Telfairic acid **L49**
 telluric acid, disodium salt **S95**
 telluric chloride **T18**
 tellurium **T16**
 tellurium diethyldithiocarbamate **E174**
 tellurium hexafluoride **T17**
 tellurium tetrachloride **T18**
 tellurium tetrakis(diethyl dithiocarbamate) **E174**
 tellurobismuthite **B132**
 Telodrin **I82**
 Telok **N206**
 Telvar **M350**
 Telvar Monuron Weed Killer **M350**
 Temasept IV **T208**
 Temed **T89**
 temephos **T19**
 temik **A62**
 Tempest **E72**
 Tenalin **M117**
 Tenite 800 **P224**
 Tennecatin **P191**
 Tenox PG **P332**
 Tensaryl SB Ca **C32**
 Tenuate **D316**
 TEPA **T346**
 TEP-HP **T288**
 TEPP **T68**
 terbacil **T20**
 terbenzene **T28**
 Terbine **C141**
 terbium **T21**
 terbufos **T22**
 terbumeton **T23**
 terbuthylazine **T24**
 Terbutrex **T25**
 terbutryn **T25**
 terephthalic acid **T26**
 terephthalonitrile **T27**
 terephthalyl alcohol bis(chloromethyl) ether **B122**
 Tergitol XH **P218**
 Teridox **D371**
 Terinin **P16**
 Termini-Ded **C118**
 Tern **F19**
 1,4(8)-terpadiene **T37**
 Terpan **C343**
 terpene polychlorinate **P221**
 terphenyl **T28**
 1,1':2',1''-terphenyl **T30**
 1,1':4',1''-terphenyl **T31**
 1,3-terphenyl **T29**
m-terphenyl **T29**
o-terphenyl **T30**
p-terphenyl **T31**
 terpin **T32**
 1,8-terpin **T32**
cis-1,8-terpin **T33**
 α -terpinene **T34**
 terpineol **T35**
 Terpineol 318 **T35**
 α -terpineol **T36**
 terpineol schlechthin **T36**
 terpinol **T35**
 terpinolene **T37**
 Terra Alba 114836 **C45**
 Terrachlor **Q12**
 terrafungine **O64**
 Terrazole **E185**
 tertiary calcium phosphate **C40**
 testandrone **T38**
 testosterone **T38**
trans-testosterone **T38**
 testosterone hydrate **T38**
 testoviron **T38**
 TETA **T284**
 tetacin-calcium **E4**
 tetraaluminium tricarbide **A98**
 tetraamminecopper(2+) sulfate (1:1) **C443**
 tetraamminecopper(II) sulfate **C443**
 1,4,7,10-tetraazadecane **T284**
 1,5,10,14-tetraazatetradecane **S107**
 3,6,9,12-tetraazatetradecane-1,14-diamine **P38**
 tetrabarium heptasulfide **B23**
 tetrabase **M212**
 Tetrabon **T62**
 tetrabromide methane **C77**
 tetrabromobisphenol A **T39**
 tetrabromodihydroxydiphenylpropane **T39**
 2',4',5',7'-tetrabromo-3',6'-dihydroxyspiro [isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, disodium salt **E29**
 1,1,2,2-tetrabromoethane **T40**
sym-tetrabromoethane **T40**
 tetrabromofluorescein **E29**
 2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol **T39**
 tetrabromomethane **C77**
 tetra(bromomethyl)methane **P37**
 tetrabromoneopentane **P37**
 tetrabutylammonium hydroxide **T41**
 5,5,12,12-tetrabutyl-7,10-dioxo-6,11-dioxa-5,12-distannahexadec-8-ene **T216**
 tetrabutylstannane **T42**
 tetrabutyltin **T42**
 tetra-*N*-butyltin **T42**
 Tetracap **T51**
 tetracarbonylhydrocobalt **C374**
 tetracarbonylnickel **N51**
 tetracene **N6**
 tetrachlor-*p*-benzoquinone **C115**
 tetrachloroacetone **T43**
 1,1,3,3-tetrachloroacetone **T43**
 tetrachloroanisole **T53**
 tetrachlorobenzene **T46**

tetrachlorobenzene **T45**
 tetrachlorobenzene **T44**
 1,2,3,4-tetrachlorobenzene **T44**
 1,2,3,5-tetrachlorobenzene **T45**
 1,2,4,5-tetrachlorobenzene **T46**
 2,3,5,6-tetrachloro-1,4-benzenedicarboxylic acid, dimethyl ester **C317**
 2,3,5,6-tetrachloro-1,4-benzoquinone **C115**
 2,3,5,6-tetrachloro-2,5-cyclohexadiene-1,4-dione **C115**
 tetrachlorocyclopentadiene **T47**
 1,2,3,4-tetrachloro-1,3-cyclopentadiene **T47**
 2,3,7,8-tetrachlorodibenzo-1,4-dioxin **D110**
 2,3,7,8-tetrachlorodibenzo[*b,e*][1,4]dioxin **D110**
 tetrachlorodifluoroethane **D333**
 1,1,1,2-tetrachloro-2,2-difluoroethane **D333**
 1,1,2,2-tetrachloro-1,2-difluoroethane **D334**
 4,5,6,7-tetrachloro-3',6'-dihydroxy-2',4',5',7'-tetraiodospiro-[isobenzofuran-1(3*H*), 9'[9*H*]*x*anthen]-3-one, disodium salt **R16**
 tetrachlorodiphenylethane **D30**
 2,4,5,4'-tetrachlorodiphenyl sulfone **T63**
 tetrachloroethane **T50**
 tetrachloroethane **T48**
 tetrachloroethane **T49**
 1,1,1,2-tetrachloroethane **T49**
 1,1,2,2-tetrachloroethane **T50**
 1,2,2,2-tetrachloroethane **T49**
sym-tetrachloroethane **T50**
 tetrachloroethene **T51**
 tetrachloroethylene **T51**
 tetrachloroethyleneum **T51**
N-1,1,2,2-tetrachloroethylmercapto-4-cyclohexene-1,2-carboximide **C58**
 2,3,4,5-tetrachlorohydroxybenzene **T54**
 4,5,6,7-tetrachloro-1(3*H*)-isobenzofuranone **P174**
 tetrachloroisophthalonitrile **C286**
 tetrachlorometaphthalodinitrile **C286**
 tetrachloromethane **C78**
 1,2,4,5-tetrachloro-3-methoxy-6-nitrobenzene **T53**
 2,3,5,6-tetrachloro-4-(methylsulfonyl)pyridine **T52**
 2,3,5,6-tetrachloro-4-nitroanisole **T53**
 1,2,4,5-tetrachloro-3-nitrobenzene **T14**
 2,3,5,6-tetrachloro-1-nitrobenzene **T14**
 tetrachlorophenol **T56**
 tetrachlorophenol **T55**
 tetrachlorophenol **T54**
 2,3,4,5-tetrachlorophenol **T54**
 2,3,4,6-tetrachlorophenol **T55**
 2,3,5,6-tetrachlorophenol **T56**
 2,4,5,6-tetrachlorophenol **T55**
 4,5,6,7-tetrachlorophthalide **P174**
m-tetrachlorophthalodinitrile **C286**
 1,1,1,3-tetrachloropropane **T57**
 1,2,2,3-tetrachloropropane **T58**
 1,1,3,3-tetrachloro-2-propanone **T43**
 tetrachloropropene **T59**
 1,1,2,3-tetrachloropropene **T59**
 tetrachloroquinone **C115**
 tetrachlorostannane **T160**
 4,5,6,7-tetrachloro-2',4',5',7'-tetraiodofluorescein, disodium salt **R16**
 tetrachlorothorium **T149**
 tetrachlorotin **T160**
 tetrachlorotitanium **T166**
 $\alpha,\alpha,\alpha,2$ -tetrachlorotoluene **C166**
 $\alpha,\alpha,\alpha,4$ -tetrachlorotoluene **C167**
o, α,α,α -tetrachlorotoluene **C166**
p- α,α,α -tetrachlorotoluene **C167**
 tetrachlorvinphos **T60**
 tetraconazole **T61**
 2,6,10,14,18,22-tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (*all-E*)- **S109**
 tetracycline **T62**
 tetracycline methylenelysine **L66**
 tetradecahydrodecaborane **D37**
 tetradecanal **M363**
 tetradecanoic acid **M362**
n-tetradecanoic acid **M362**
 1-tetradecyl aldehyde **M363**
 tetradecyloxirane **E37**
 tetradifon **T63**
 tetraethoxysilane **T67**
 tetraethylene glycol **T64**
 tetraethylenepentamine **T65**
 tetraethyllead **T66**
 tetraethyl orthosilicate **T67**
 tetraethylplumbane **T66**
 tetraethyl pyrophosphate **T68**
 tetraethylrhodamine **R9**
 tetraethyl silicate **T67**
 tetraethylstannane **T69**
 tetraethylthioperoxydicarbonic diamide **D565**
 tetraethylthiuram disulfide **D565**
 tetraethyltin **T69**
 Tetrafil **T62**
 tetrafluoroboric acid **F46**
 tetrafluoroethene **T70**
 tetrafluoroethylene **T70**
 1,1,2,2-tetrafluoroethylene **T70**
 tetrafluoroethylene homopolymer **P232**
 tetrafluoromethane **C79**
 2,3,5,6-tetrafluoro-4-methylbenzyl (*Z*)-(1*RS*, 3*RS*)-3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethylcyclopropanecarboxylate **T15**
 [1 α ,3 α (*Z*)]-(\pm)-(2,3,5,6-tetrafluoro-4-methylphenyl)methyl **T15**
 tetrafluorosulfurane **S156**
 1,2,3,6-tetrahydrobenzaldehyde **T71**
 1,2,5,6-tetrahydrobenzaldehyde **T71**
 tetrahydrobenzene **C511**
 1,2,3,4-tetrahydrobenzene **C511**
 [2*R*-(2 α ,6 α ,12 α)]-1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-[1]benzopyrano-[3,4-*b*]furo[2,3-*h*][1]benzopyran-6(6*aH*)-one **R18**

tetrahydro-5,5-dimethyl-2(1*H*)-pyrimidinone, [3-[4-(trifluoromethyl)phenyl]-1-[2-[4-(trifluoromethyl)phenyl]ethenyl]-2-propenylidene]hydrazone **H86**
 tetrahydro-3,5-dimethyl-2*H*-1,3,5-thiadiazine-2-thione **D24**
 tetrahydro-2,5-dioxofuran **S129**
 1,2,3,6-tetrahydro-2,6-dioxo-4-pyrimidinecarboxylic acid **O34**
 tetrahydrofuran **T72**
 tetrahydro-2-furan carbinol **T74**
 2,5-tetrahydrofuran dimethanol **T73**
 tetrahydro-2,5-furandione **S129**
 tetrahydrofuran-2,5-diyl dimethanol **T73**
 tetrahydro-2-furanmethanamine **T75**
 tetrahydro-2-furanmethanol **T74**
 tetrahydrofurfuryl alcohol **T74**
 tetrahydrofurfurylamine **T75**
 tetrahydro-2-furylmethanol **T74**
 tetrahydrogermane **G13**
 2,3,6a,9a-tetrahydro-9a-hydroxy-4-methoxycyclopenta-[c]furo[3',2':4,5]furo[2,3-*h*]benzopyran-1,11-dione **A57**
 [(1*S*-(1 α ,6 β ,9 α , β))-2,3,6a,9a-tetrahydro-1-hydroxy-4-methoxycyclopenta[*c*]furo[3',2':4,5]furo[2,3-*h*][1]benzopyran-11(1*H*)-one **A52**
 3a,4,7,7a-tetrahydro-5-(hydroxyphenyl-2-pyridinylmethyl)-phenyl-2-pyridinylmethylene-4,7-methano-1*H*-isoindole-1,3(2*H*)-dione **N201**
 3a,4,7,7a-Tetrahydro-4,7-methano-1*H*-indene **D271**
 3,4,7 α ,10 α -tetrahydro-5-methoxy-1*H*,12*H*-furo[3',2':4,5]-furo[2,3-*h*]pyranol[3,4-*c*][1]benzopyran-1,12-dione **A55**
 tetrahydro-2-methylfuran **M308**
 tetrahydro-5-methyl-2-furanone **V3**
 2,3,4,5-tetrahydro-2-methyl-5-(phenylmethyl)-1*H*-pyrido[4,3-*b*]indole **M36**
 1,2,3,4-tetrahydronaphthalene **T80**
 1,2,3,4-tetrahydro-1-naphthyl hydroperoxide **T81**
 tetrahydro-*N*-nitrosopyrrole **N174**
 tetrahydro-1,4-oxazine **M353**
 tetrahydro-*p*-oxazine **M353**
 tetrahydrophthalic acid anhydride **T76**
 tetrahydrophthalic anhydride **T76**
N-(3,4,5,6-tetrahydrophthalimide)methyl *cis/trans*-chrysanthemate **T85**
 tetrahydropyrrole **P367**
 1,2,5,6-tetrahydro-4*H*-pyrrolo[3,2,1-*ij*]quinolin-4-one **P365**
 1,2,3,4-tetrahydrostyrene **V31**
 tetrahydrosylvan **M308**
 5,6,6a,7-tetrahydro-1,2,9,10-tetramethoxy-6-methyl-4*H*-dibenzo[*de,g*]quinoline **G15**
 (*S*)-*N*-(5,6,7,9-tetrahydro-1,2,3,10-tetramethoxy-9-oxobenzo-[*a*]heptalen-7-yl)acetamide **C384**
 tetrahydrothiophene **T77**
 tetrahydrothiophene 1,1-dioxide **S143**
 2,2',4,4'-tetrahydroxybenzophenone **T78**
 tetrahydroxymethylmethane **P35**
 tetrahydroxymethylphosphonium chloride **T79**
 3,3',5,5'-tetraiodothyronine **T156**
 tetrakis(bromomethyl)methane **P37**
 tetrakis(diethylcarbomodithioato-*S,S'*)selenium **S15**
 tetrakis(diethylcarbomodithioato-*S,S'*)tellurium **E174**
 tetrakis(hydroxymethyl)methane **P35**
 tetrakis(hydroxymethyl)phosphonium chloride **T79**
 Tetralex **T51**
 tetralin **T80**
 tetralin hydroperoxide **T81**
 tetralon **T82**
 tetralone **T82**
 1-tetralone **T83**
 2-tetralone **T84**
 α -tetralone **T83**
 β -tetralone **T84**
 tetralyl hydroperoxide **T81**
 1,2,9,10-tetramethoxyaporphine **G15**
 6',7',10,11-tetramethoxyemetan dihydrochloride **E17**
 tetramethoxysilane **T91**
 tetramethrin **T85**
N,N,N',N'-tetramethyl-3,6-acridinediamine **C421**
 tetramethylammonium hydroxide **T86**
 1,2,3,4-tetramethylbenzene **T87**
 1,2,3,5-tetramethylbenzene **T88**
 1,2,4,5-tetramethylbenzene **D602**
N,N,N',N'-tetramethyl-1,4-benzenediamine **T92**
exo-1,2,7,7-tetramethylbicyclo[2.2.1]-heptan-2-ol **M240**
 1,3,5,8-tetramethyl-2,4-bis(α -hydroxyethyl)porphine-6,7-dipropionic acid **H13**
 (1,1,3,3-tetramethylbutyl)phenol **O23**
 α -[4-(1,1,3,3-tetramethylbutyl)phenyl]- ω -hydroxypoly(oxy-1,2-ethanedyl) **O20**
 tetramethyldiaminobenzophenone **B128**
 tetramethyldiaminodiphenylacetimine **A254**
 tetramethyldiaminodiphenylmethane **M212**
 3,7,9,13-tetramethyl-5,11-dioxo-2,8,14-trithia-4,7,9,12-tetraazapentadeca-3,12-diene-6,10-dione **T128**
 tetramethylene cyanide **A49**
 tetramethylene diacrylate **B207**
 tetramethylenediamine **B201**
 tetramethylene glycol **B204**
 1,4-tetramethylene glycol **B204**
 tetramethylene oxide **T72**
 tetramethylene sulfide **T77**
 tetramethylenimine **P367**
N,N,N',N'-tetramethyl-1,2-ethanediamine **T89**
N,N,N',N'-tetramethylethylenediamine **T89**
 tetramethyllead **T90**
 tetramethylmethane **N39**
 tetramethylolmethane **P35**
 tetramethylolmethane tetracrylate **P36**
 tetramethyl orthosilicate **T91**
N,N,N',N'-tetramethyl-*p*-phenylenediamine **T92**
 tetramethylphosphorodiamidic fluoride **D367**
N,N,N',N'-tetramethylphosphorodiamidic fluoride **D367**
 tetramethylplumbane **T90**
 tetramethylsilane **T93**
 tetramethyl silicate **T91**

1'-2,C-4,C-6,C-8-tetramethyl-1,3,5,7-tetroxocane **M94**
 2,4,6,8-tetramethyl-1,3,5,7-tetroxocane **M94**
O,O,O',O'-tetramethyl *O,O'*-thiodi-*p*-phenylenedi-
 phosphorothioate **T19**
 tetramethylthionine chloride **M216**
 tetramethylthioperoxydicarbonic diamide **T147**
 tetramethylthiuram disulfide **T147**
 tetramethylthiurammonium sulfide **M348**
 Tetran **C535**
 Tetranap **T80**
 1,2,3,4-tetranitrocarbazole **T94**
 tetranitromethane **T95**
 2,5,8,11-tetraoxadodecane **T296**
 2,2'-(2,5,8,11-tetraoxa-1,12-dodecanediyl)bisoxirane **T282**
 tetraphene **B43**
 tetraphosphoric acid, hexaethyl ester **H44**
 tetraphosphorus trisulfide **P164**
 tetrapropyl dithiopyrophosphate **T96**
O,O,O,O-tetrapropyl dithiopyrophosphate **T96**
 tetrapropyl orthotitanate **T97**
 tetrasodium diphosphate **S88**
 tetrasodium ethylenediaminetetraacetate **E8**
 tetrasodium pyrophosphate **S88**
 tetrasul **T98**
 tetrazobenzene- β -naphthol **C422**
 tetrole **F123**
 Tetropil **T51**
 Tetrosan 3,4D **A67**
 tetrosin P300 **P127**
 Tetryl **N65**
 tetryl formate **I90**
 Texacat DME **D388**
 Texanol isobutyrate **T316**
 Texapon K12 **S76**
 Texlin 300 **T284**
 Textile Red WD-263 **C417**
 Textone **S54**
 TFE **T70**
 téfluthrine **T15**
 thalidomide **T99**
 Thalitone **C318**
 thallium **T100**
 thallium(I) acetate **T101**
 thallium(1+) carbonate **T102**
 thallium(I) carbonate **T102**
 thallium(I) chloride **T103**
 thallium hydrogen sulfate **T104**
 thallium(I) malonate **T105**
 thallium(I) methanoate **T101**
 thallium monochloride **T103**
 thallium mononitrate **T106**
 thallium(I) nitrate **T106**
 thallium(3+) oxide **T107**
 thallium(III) oxide **T107**
 thallium(III) oxide **T107**
 thallium peroxide **T107**
 thallium sesquioxide **T107**

thallium(I) sulfate **T108**
 thalious acetate **T101**
 thalious carbonate **T102**
 thalious chloride **T103**
 thalious malonate **T105**
 thalious nitrate **T106**
 thalious sulfate **T108**
 Tham **T356**
 Thanate P 210 **P114**
 THBP **T78**
 Theelol **O25**
 thenylene hydrochloride **M118**
 thenylpyramine **M117**
 thenylpyramine hydrochloride **M118**
 theobromine **T109**
 Theoharn **M47**
 theophylline **T110**
 Thermacure **M222**
 Thermphos **S98**
 Thesal **T109**
 THF **T72**
 THFA **T74**
 THF glycol **T73**
 4-thia-1-azabicyclo(3.2.0)heptane-2-carboxylic acid, 6-
 ((amino(4-hydroxyphenyl)acetyl)amino)-3,3-dimethyl-7-
 oxo, (2*S*-(2 α ,5 α ,6 β (*S*)+))- **A192**
 4-thia-1-azabicyclo(3.3.0)heptane-2-carboxylic acid, 6-
 ((aminophenylacetyl)amino)-3,3-dimethyl-7-oxo-2,
 (5-12 α ,5 α ,6 β 7(*S*+)) **A194**
 4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-
 dimethyl-7-oxo-6-[(phenylacetyl)amino]-[2*S*(2 α 6 β)-,
 compound with *N,N'*-bis(phenylmethyl)-1,2-
 ethanediamine (2:1) **B46**
 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-
 [(aminophenylacetyl)amino]-3-methyl-8-oxo-[6*R*-
 [6 α ,7 β *R*]] **C100**
 1-thia-3-azaindene **B76**
 thiabenzazole **T111**
 7-thia-7(H)-benzo[*c*]fluorene **B65**
 thiacetamide **T115**
 thiactic acid **T116**
 thiacyclopentadiene **T139**
 thiacyclopentane **T77**
 1-thia-3-cyclopentene 1,1-dioxide **S144**
 thiacyclopropane **E121**
 4*H*-1,3,5-thiadiazin-4-one, 2-[(1,1-dimethylethyl)imino]-
 tetrahydro-3-(1-methylethyl)-5-phenyl- **B194**
 2-thiaindone **D343**
 thialane **T77**
 Thiamazole **M122**
 thiamin **T112**
 thiamine **T112**
 thiamine chloride **T112**
 thiamine chloride hydrochloride **T113**
 thiamine dichloride **T113**
 thiamine hydrochloride **T113**
 thiaminium chloride hydrochloride **T113**

3-thiapentane **E172**
 2-thiapropane **D456**
 thiate E **T326**
 thiazole **T114**
 2-(3*H*)-thiazolone, 4-(5-nitro-2-furanyl)-, dimethylhydrazone **D423**
 2-[[[4-[(2-thiazolylamino)sulfonyl]phenyl]amino]carbonyl]-benzoic acid **P177**
 2-(thiazol-4-yl)benzimidazole **T111**
 4'-(2-thiazolylsulfamyl)phthalanilic acid **P177**
 thiglycolic acid, methyl ester **M248**
 thiirane **E121**
 Thimerosal **T133**
 Thimet **P145**
 thioacetamide **T115**
 thioacetic acid **T116**
 Thioallate **S135**
 thioamidodicarbonic diamide **D574**
 thioaniline **T127**
 thiobencarb **T117**
 2,2'-thiobisacetic acid **T130**
 4,4'-thiobisbenzenamine **T127**
 4,4'-thiobis(5-*tert*-butyl-*m*-cresol) **T118**
 4,4'-thiobis(5-*tert*-butyl-*o*-cresol) **T119**
 4,4'-thiobis(2-*tert*-butyl-6-methylphenol) **T118**
 4,4'-thiobis(6-*tert*-butyl-3-methylphenol) **T118**
 6,6'-thiobis(4-chloro-*o*-cresol) **T120**
 1,1'-thiobis[2-chloroethane] **M359**
 2,2'-thiobis(4-chloro-6-methylphenol) **T120**
 2,2'-thiobis(4-chlorophenol) **T121**
 2,2'-thiobis(4,6-dichlorophenol) **T122**
 2,2'-thiobis[4,6-dichloro-phenol, disodium salt] **S49**
 thiobis[(4,6-dichloro-*o*-phenylene)oxy]disodium **S49**
 4,4'-thiobis[3-(1,1-dimethylethyl)-6-methylphenol] **T119**
 1,1'-thiobis(*N,N*-dimethylthio)formamide **M348**
 thiobis(dodecyl propionate) **D365**
 1,1'-thiobisethane **E172**
 thiobismethane **D456**
 1,1'-thiobis(2-methyl-4-hydroxy-6-*tert*-butylbenzene) **T118**
 3,3'-thiobispropanoic acid, didodecyl ester **D365**
 thiobutyl alcohol **B211**
 thiocarbamide **T146**
 thiocarbamoylhydrazine **T144**
 thiocarbanil **P115**
 thiocarbanilide **T123**
 thiocarbazine **T124**
 thiocarbazil **T162**
 thiocarbohydrazide **T124**
 thiocarbonic dichloride **T140**
 thiocarbonic dihydrazide **T124**
 thiocarbonohydrazide **T124**
 thiocarbonyl dichloride **T140**
 thiocyanatoethane **E175**
 2-(thiocyanatomethylthio)benzothiazole **T125**
 2-[(thiocyanatomethylthio)benzothiazole **T125**
 thiocyanic acid, ammonium salt **A190**
 thiocyanic acid, ethyl ester **E175**
 thiocyanic acid, lead salt **L33**
 thiocyanic acid mercury(2+) salt **M87**
 thiocyanuric acid, (2-benzothiazolyl(thio))methyl ester **T125**
 thiocyclam hydrogen oxalate **T126**
 Thiodan II **E20**
 Thiodan sulfate **E21**
 thiodemeton **D566**
 thiodiacetic acid **T130**
 4,4'-thiodianiline **T127**
 thiodicarb **T128**
 thiodicarbonic diamide ((H₂(N)C(S))₂S), tetramethyl- **M348**
 2,2'-thiodiethanoic acid **T130**
 2,2'-thiodiethanol **T129**
 thiodiethylene glycol **T129**
 β-thiodiglycol **T129**
 thiodiglycolic acid **T130**
 thiodiphenylamine **P83**
O,O'-(thiodi-4,1-phenylene) bis(*O,O'*-dimethylphosphorothioate) **T19**
 thiodi-*p*-phenylenediamine **T127**
O,O'-thiodi-*p*-phenylene *O,O,O',O'*-tetramethyl bis(phosphorothioate) **T19**
 thiodiphosphoric acid, *O,O,O',O'*-tetraethyl ester **S147**
 thioethanol **E60**
 2-thioethanol **M62**
 thioethyl ether **E172**
 thiofanocarb **T131**
 thiofanox **T131**
 Thiofax **Z10**
 thiofuran **T139**
 thiofurfuran **T139**
 (1-thio-D-glucopyranosato)-gold **A255**
 1-thio-glucopyranose, monogold(I) salt **A255**
 thioglycol **M62**
 thioglycolic acid **M59**
 thioglycolic acid 2-ethylhexyl ester **E134**
 2-thioindan **D343**
 thiolacetic acid **T116**
 thiolactic acid **T132**
 thiole **T139**
 thiomersal **T133**
 Thiomersalate **T133**
 thiomethyl alcohol **M115**
 thiometon **T134**
 thionaphthalene **B77**
 thionaphthene **B77**
 thionazin **T135**
 α-Thionex **E20**
 thionoacetic acid **T116**
 Thionylan **M117**
 thionyl chloride **T136**
 thionyl dichloride **T136**
 thiophanate **T137**
 thiophanate-methyl **T138**

Thiophane **T77**
 thiophan sulfone **S143**
 thiophene **T139**
 thiophenol **B50**
 Thiophos **P13**
 thiophosgene **T140**
 thiophosphoric anhydride **P162**
 thiophosphoryl chloride **T141**
 2-thiopseudourea **T146**
 β -thiopseudourea **T146**
 6-thiopurine **M63**
 thiopyrophosphoric acid, tetraethyl ester **S147**
 thioquinox **T142**
 thioridazine **T143**
 thiosemicarbazide **T144**
 thiosemicarbazone acetone **A19**
 thiosinamine **A93**
 Thiosol **S149**
 Thiostop E **D575**
 thiosulfuric acid, diammonium salt **A191**
 thio-TEPA **T347**
 thioteppe **S147**
 thiotetrole **T139**
 2-thio-1-(thiocarbamoyl)urea **D574**
 Thiothymin **M312**
 2-thio-1-*o*-tolylurea **T193**
 thiouracil **T145**
 2-thiouracil **T145**
 thiourea **T146**
 2-thiourea **T146**
 Thiovanic Acid **M59**
 thioxamyl **O47**
 thiram **T147**
 Thiurad **T147**
 thoria **T150**
 thorium **T148**
 thorium chloride **T149**
 thorium dioxide **T150**
 thorium nitrate **T151**
 thorium(4+) nitrate **T151**
 thorium oxide **T150**
 thorium(IV) oxide **T150**
 thorium tetrachloride **T149**
 thorium tetranitrate **T151**
 T₄(hormone) **T156**
 thorotrast **T150**
 THPC **T79**
 L-threitol (2S,3S)-1,4-dimethanesulfonate **T195**
 L-threonine **T152**
 Threosulphan **T195**
 T-Hydro **B261**
 thyme camphor **T154**
 Thymidazole **M122**
 thymine **T153**
 thymine (pure base) **T153**
 thymol **T154**
m-thymol **T154**

thymoxamine **T155**
 Thyreoideum **T156**
 Thyreostat II **P337**
 Thyroxinal **T156**
 L-thyroxine **T156**
 Ti 160 **T164**
 Tigason **E184**
 tiglic acid **T157**
 Tiguvon **F24**
 Tillam **P17**
 Tilt **P306**
 Timonil **C61**
 tin **T158**
 tin bifluoride **T161**
 tin(II) chloride **T159**
 tin(IV) chloride **T160**
 tin dichloride **T159**
 tin difluoride **T161**
 tin flake **T158**
 tin(II) fluoride **T161**
 tin powder **T158**
 tin tetrachloride **T160**
 Tintorane **W3**
 tintriphenyl acetate **F25**
 tiocarbazil **T162**
 Tiolent **C498**
 Tiona RCL-376 **T165**
 Tioxide **T165**
 Tioxide AD-M **T165**
 Tip-Nip **U5**
 Ti-Pure **T165**
 tirpate **T163**
 Tisperse MB-58 **Z10**
 titanium **T164**
 titanium(III) chloride **T167**
 titanium(IV) chloride **T166**
 titanium chloride (TiCl₃) **T167**
 titanium chloride (TiCl₄) (T-4)- **T166**
 titanium dioxide **T165**
 titanium(IV) oxide **T165**
 titanium peroxide **T165**
 titanium(IV) propoxide **T97**
 titanium tetrachloride **T166**
 titanium trichloride **T167**
 titanocene dichloride **T168**
 titanous chloride **T167**
 Tixit **P305**
 TKB **N154**
 TL-1380 **P179**
 TL 1070 **C8**
 TL 214 **E112**
 TL 337 **A266**
 TL 797 **V38**
 TMA **T299**
 TMA **T303**
 TMID **T147**
 TMOS **T91**

TMP **T324**
 TMPD **E116**
 TMPD **T92**
 TMPD (alcohol) **T315**
 TMPTA **T311**
 TNB **T329**
 TNF **T330**
 TNM **T95**
 T-Nox **T1**
 TNT **T331**
 Tobago **B232**
 (2*R*,4'*R*,8'*R*)- α -tocopherol **T169**
 α -tocopherol **T169**
 Tof **T355**
 Tofranil **I15**
 Tofuron **F132**
 Tok **N112**
 Tokokin **E53**
 Tokuthion **P341**
 tolanase **T170**
 tolazamide **T170**
 tolbutamide **T171**
 Toleron **I72**
 3,3'-tolidine **T172**
 o-tolidine **T172**
 tolinase **T170**
 Tolit **T331**
 Tolkan **I133**
 Tolonate **H55**
 toluazotoluidine **C424**
 toluene **T173**
 toluene-2-azonaphthol-2 **O27**
 o-toluenecarbonitrile **T189**
 toluene-2,3-diamine **D86**
 toluene-2,4-diamine **D87**
 2,3-toluenediamine **D86**
 2,4-toluenediamine **D87**
 2,5-toluenediamine **D88**
 2,6-toluenediamine **D90**
 3,4-toluenediamine **D92**
 o-toluenediamine **D86**
 p-toluenediamine **D88**
 2,5-toluenediamine hemisulfate **D89**
 2,5-toluenediamine sulfate **T174**
 p-toluenediamine sulfate **D89**
 toluene diisocyanate **T175**
 toluene 2,4-diisocyanate **T176**
 2,4-toluene diisocyanate **T176**
 toluene 2,6-diisocyanate **T177**
 2,6-toluene diisocyanate **T177**
 toluene hexahydride **M197**
 p-toluene isocyanate **T192**
 p-toluenenitrile **T190**
 toluene-4-sulfonamide **T178**
 4-toluenesulfonamide **T178**
 p-toluenesulfonamide **T178**
 p-toluenesulfonic acid **T179**

p-toluenesulfonic acid, methyl ester **M313**
 toluene-4-sulfonyl chloride **T180**
 p-toluenesulfonyl chloride **T180**
 4-toluic acid **T183**
 m-toluic acid **T181**
 o-toluic acid **T182**
 p-toluic acid **T183**
 m-toluic acid, diethylamide **D319**
 p-toluic nitrile **T190**
 2-toluidine **T185**
 m-toluidine **T184**
 o-toluidine **T185**
 p-toluidine **T187**
 o-toluidine hydrochloride **T186**
 Toluidine Red **C416**
 m-toluidine, α,α,α -trifluoro- **A118**
 o-toluidinium hydrochloride **T186**
 α -tolunitrile **B97**
 m-tolunitrile **T188**
 o-tolunitrile **T189**
 p-tolunitrile **T190**
 toluol **T173**
 m-toluol **C457**
 o-toluol **C458**
 p-toluol **C459**
 m-toluquinoline **M302**
 p-toluquinoline **M301**
 m-toluylic acid **T181**
 o-toluylic acid **T182**
 m-tolylamine **T184**
 o-tolylamine **T185**
 p-tolylamine **T187**
 o-tolylazo- β -naphthol **O27**
 4-(o-tolylazo)-o-toluidine **C424**
 tolyl chloride **B95**
 m-tolyl chloride **C289**
 o-tolyl chloride **C288**
 p-tolyl chloride **C290**
 3,5-tolylenediamine **D93**
 m-tolylenediamine **D87**
 tolylene 2,4-diisocyanate **T176**
 tolylene 2,6-diisocyanate **T177**
 m-tolylene 2,6-diisocyanate **T177**
 tolylene isocyanate **T175**
 1-(p-tolyl)ethanol **D402**
 tolyl ethylene **M306**
 tolylfluorid **T191**
 tolyl glycidyl ether **C460**
 4-tolyl isocyanate **T192**
 p-tolyl isocyanate **T192**
 m-tolyl methyl carbamate **M324**
 p-tolylmethylcarbinol **D402**
 p-tolyl methyl ether **M157**
 m-tolyl nitrile **T188**
 o-tolyl nitrile **T189**
 p-tolyl nitrile **T190**
 p-tolylsulfonic acid **T179**

p-tolylsulfonyl chloride **T180**
N-(*o*-tolyl)thiourea **T193**
o-tolylthiourea **T193**
 tolyltriazole **M164**
 Tomatone **C452**
 Tomatotone **C452**
 Tomlinite **L42**
 Tomorin **C445**
 Tonka bean camphor **C447**
 Topanol **D405**
 Topaze **P18**
 Topflor **F89**
 Topitox **C238**
 Toprose **F105**
 Torak **D68**
 Torbin **E40**
 Tordon **P182**
 torporex **P231**
 Torque **F7**
 Torus **F17**
 tosoic acid **T179**
 tosylchloramide sodium **C113**
 tosyl chloride **T180**
 Toterbane **D579**
 Tough **P356**
 toxaphene **C48**
 toxicilic acid **M12**
 Toxicilic anhydride **M13**
 Toyocat-DMA **D388**
 Toyocat-DMCH **D411**
 Toyodan **P341**
 TPIA **N2**
 TPP **T337**
 TPP **T339**
 TPTA **F25**
 TPTH **F26**
 TPT-MA **T312**
 Tracker **T194**
 tragacol **L57**
 Tralate **T194**
 tralomethrin **T194**
 tralométhrine **T194**
 Tralox **T194**
 Tramet **E72**
 (3*R*-*trans*)-4,6-dihydro-8-hydroxy-3,4,5-trimethyl-6-oxo-3*H*-
 2-benzopyran-7-carboxylic acid **C353**
 Transflo **F4**
 Trapex **M245**
 Trapp **B196**
 Trastan **F88**
 Trecator-SC **E69**
 Trenimon **T345**
 treosulfan **T195**
 Trescatyl **E69**
 Tret-o-lite XC511 **A66**
 triacetin **T196**
 triacetyl glycerin **T196**
 triacylglycerol hydrolase **L51**
 triadimenol **T197**
 Triadine 3 **H51**
 Triafur **A137**
 tri-allate **T198**
 triallylamine **T199**
 tri-*N*-allylamine **T199**
 triallyl borate **T200**
 triallyl isocyanurate **T201**
 triallyl-1,3,5-triazine-2,4,6-(1*H*,3*H*,5*H*)-trione **T201**
 2,4,7-triamino-6-phenylpteridine **T203**
 2,4,6-triaminotriazine **M47**
 triamiphos **T202**
 Triampur **T203**
 triamterene **T203**
 tri-*p*-anisylchloroethylene **C299**
 triatomic oxygen **O65**
 Triatox **A158**
 1,5,10-triazadecane **S106**
 3,5,7-triazaindole **P346**
 3,6,9-triazaundecamethylenediamine **T65**
 3,6,9-triazaundecane-1,11-diamine **T65**
 Triazine **A208**
s-triazine, 2-chloro-4,6-bis(isopropylamino)- **P302**
s-triazine, 2-chloro-4-(diethylamino)-6-(ethylamino)- **T275**
 1,3,5-triazine-2,4-diamine, 6-chloro-*N,N'*-bis(1-
 methylethyl)- **P302**
 1,3,5-triazine-2,4-diamine, *N*-ethyl-*N'*-(1-methylethyl)-6-
 (methylthio)- **A109**
 1,3,5-triazine-2,4-diamine, 6-(5-nitro-2-furanyl)- **D80**
 1,3,5-triazine-2,4,6-triamine **M47**
 1,3,5-triazine-2,4,6-triamine, *N*-cyclopropyl- **C545**
 1,3,5-triazine-1,3,5-(2*H*,4*H*,6*H*)-triethanol **H51**
s-triazine, 2,4,6-trifluoro- **C493**
s-triazinetriol **C491**
s-triazine-2,4,6-(1*H*,3*H*,5*H*)-trione **C491**
 triaziquone **T345**
 triazoic acid **H97**
 1,2,4-triazole **T204**
 1*H*-1,2,4-triazole **T204**
 1*H*-1,2,4-triazole-1-ethanol, β-[(2,4-dichlorophenyl)-
 methylene]-α-(1,1-dimethylethyl)-, (*E*)- **D464**
 1*H*-1,2,4-triazole-1-propanenitrile, α-butyl-α-(4-
 chlorophenyl)- **M360**
 1*H*-1,2,4-triazol-3-ylamine **A160**
 (1*H*-1,2,4-triazolyl)tricyclohexyl stannane **A270**
 (1*H*-1,2,4-triazolyl-1-yl)tricyclohexyl stannane **A270**
 triazophos **T205**
 Tribac **T10**
 Tri-ban **P193**
 tribasic copper mixture **B142**
 Triben **T10**
 tribromoaluminium **A97**
 tribromoborane **B145**
 tribromoboron **B145**
 tribromomethane **B177**
 tribromonitromethane **T206**

2,4,6-tribromophenol **T207**
 tribromophosphine **P165**
 tribromosalan **T208**
 3,4',5-tribromosalicylanilide **T208**
 tribufos **T209**
 Tribunil **M101**
 Tribute **F28**
 tri(2-butoxyethanol phosphate) **T348**
 tributoxyethyl phosphate **T348**
 tributrin **T223**
 tributylamine **T210**
 tri-*n*-butylamine **T210**
 tributyl cellosolve phosphate **T348**
 tributyl[(2,4-dichlorophenyl)methyl]phosphonium chloride **C309**
 tributylfluorostannane **T215**
 tributyl(methacryloxy)stannane **T218**
 tributyl[(2-methyl-1-oxo-2-propenyl)oxy]stannane **T218**
 tributyl[(1-oxododecyl)oxy]stannane **T217**
 2,4,6-tri-*tert*-butylphenol **T211**
 tributyl phosphate **T212**
 tri-*n*-butyl phosphate **T212**
 tributyl phosphorotriithioate **M89**
 S,S,S-tributyl phosphorotriithioate **T209**
 tributylstannyl methacrylate **T218**
 tributyltin acetate **T213**
 tributyltin benzoate **T214**
 tributyltin dodecanoate **T217**
 tributyltin fluoride **T215**
 tributyltin fumarate **T216**
 tributyltin laurate **T217**
 tributyltin methacrylate **T218**
 tributyltin oxide **T219**
 tributyltin phthalate **T220**
 tributyltin succinate **T221**
 tributyltin sulfide **T222**
 S,S,S-tributyl trithiophosphite **M89**
 tributyrin **T223**
 tri-*n*-butyrin **T223**
 tributryl glyceride **T223**
 tricalcium arsenate **C22**
 tricalcium orthophosphate **C40**
 tricalcium phosphate **C40**
 tricaprylate **T224**
 tricaprylic glyceride **T224**
 tricaprylin **T224**
 tricarbonyl- π -cyclopentadienyl-manganese **M23**
 tricarbonyl(η^5 -2,4-cyclopentadien-1-yl)manganese **M23**
 Tri-Chlor **C259**
 trichloroacetic acid chloride **T230**
 1,1,1-trichloroethanoic acid **T226**
 trichlorfon **T225**
 Trichlormetaphos **F8**
 trichloroacetaldehyde **C107**
 trichloroacetaldehyde monohydrate **C108**
 trichloroacetic acid **T226**
 trichloroacetic acid, sodium salt **S97**
 1,1,1-trichloroacetone **T227**
 1,1,3-trichloroacetone **T228**
 α,α,α -trichloroacetone **T227**
 α,α',α' -trichloroacetone **T228**
 trichloroacetonitrile **T229**
 2,2,2-trichloroacetonitrile **T229**
 trichloroacetyl chloride **T230**
 S-2,3,3-trichloroallyl di-isopropyl(thiocarbamate) **T198**
 S-2,3,3-trichloroallyl di-isopropylthiocarbamate **T198**
 trichloroaluminium **A99**
 trichloroamylsilane **A206**
 2,3,4-trichloroaniline **T231**
 2,4,5-trichloroaniline **T232**
 2,4,6-trichloroaniline **T233**
 3,4,5-trichloroaniline **T234**
sym-trichloroaniline **T233**
 2,3,4-trichloroanisole **T235**
 2,3,5-trichloroanisole **T236**
 2,3,6-trichloroanisole **T237**
 2,4,5-trichloroanisole **T238**
 2,4,6-trichloroanisole **T239**
 trichloroarsine **A243**
 2,3,4-trichlorobenzenamine **T231**
 2,4,5-trichlorobenzenamine **T232**
 2,4,6-trichlorobenzenamine **T233**
 3,4,5-trichlorobenzenamine **T234**
 1,2,3-trichlorobenzene **T241**
 1,2,4-trichlorobenzene **T242**
 1,3,5-trichlorobenzene **T243**
sym-trichlorobenzene **T243**
unsym-trichlorobenzene **T242**
vic-trichlorobenzene **T241**
 trichlorobenzene (technical mixture) **T240**
 2,3,6-trichlorobenzoic acid **T10**
 1,1,1-trichlorobis(chlorophenyl)ethane **D35**
 1,1,1-trichloro-2,2-bis(4-chlorophenyl)ethane **D35**
 2,2,2-trichloro-1,1-bis(4-chlorophenyl)ethanol **D261**
 trichloroborane **B146**
 trichloroboron **B146**
 2,3,4-trichloro-1-butene **T244**
 trichlorobutylene oxide **T245**
 3,4,4'-trichlorocarbaniide **T270**
 trichloro(chloromethyl)silane **T246**
 1,1,1-trichloro-2-(*o*-chlorophenyl)-2-(*p*-chlorophenyl)ethane **D34**
 1,2,4-trichloro-5-[(4-chlorophenyl)sulfonyl]benzene **T63**
 1,2,4-trichloro-5-[(4-chlorophenyl)thio]benzene **T98**
 α,α,α -trichloro-4-chlorotoluene **C167**
 trichlorocyanuric acid **T250**
 trichloro-(3-cyclohexenyl)silane **C512**
 2,2,2-trichloro-1-(3,4-dichlorophenyl)ethyl acetate **P215**
 trichloro(dichlorophenyl)silane **D243**
 1,1,1-trichloro-2,2-di(4-methoxyphenyl)ethane **M132**
 3,4,4'-trichlorodiphenylurea **T270**
 1,1,1-trichloro-3,4-epoxybutane **T245**
 trichloroethanal **C107**
 1,1,1-trichloroethane **T247**

1,1,2-trichloroethane **T248**
 1,2,2-trichloroethane **T248**
 α -trichloroethane **T247**
 2,2,2-trichloro-1,1-ethanediol **C108**
 trichloroethene **T249**
 trichloroethenylsilane **V39**
 trichloroethylene **T249**
 1,1,2-trichloroethylene **T249**
 1,1'-(2,2,2-trichloroethylidene)bis(4-chlorobenzene) **D35**
 1,1'-(2,2,2-trichloroethylidene)bis(4-methoxybenzene) **M132**
 (R)-1,2-O-(2,2,2-trichloroethylidene)D-glucofuranose **C109**
 (2,2,2-trichloroethyl)oxirane **T245**
 trichloroethylsilane **E180**
 trichloroethylsilicon **E180**
 trichlorofluoromethane **F78**
 trichloroform **C201**
 trichlorohexylsilane **H79**
 trichlorohydrin **T264**
 trichloroindium **I29**
 trichloroisocyanuric acid **T250**
 trichloromelamine **T251**
 N²,N⁴,N⁶-trichloromelamine **T251**
 trichloromethanesulfonyl chloride **T252**
 1,2,3-trichloro-4-methoxybenzene **T235**
 1,2,4-trichloro-3-methoxybenzene **T237**
 1,2,4-trichloro-5-methoxybenzene **T238**
 1,2,5-trichloro-3-methoxybenzene **T236**
 1,3,5-trichloro-2-methoxybenzene **T239**
 (trichloromethyl)benzene **B79**
 1,2,4-trichloro-5-methylbenzene **T268**
 trichloromethyl cyanide **T229**
 N-trichloromethylmercapto-4-cyclohexene-1,2-dicarboximide **C59**
 N-(trichloromethylmercapto)phthalamide **F97**
 trichloromethylmethane **T247**
 trichloromethylnitrile **T229**
 trichloromethylsilane **M314**
 trichloromethylsulfonyl chloride **T252**
 2-[(trichloromethyl)thio]-1H-isoindole-1,3(2H)-dione **F97**
 N-(trichloromethylthio)phthalamide **F97**
 trichloronit **T253**
 trichloronate **T253**
 1,3,5-trichloro-2-nitrobenzene **T254**
 2,4,6-trichloronitrobenzene **T254**
 trichloronitromethane **C259**
 trichlorononylsilane **N199**
 trichlorooctadecylsilane **O4**
 trichlorooxovanadium **V11**
 trichloropentylsilane **A206**
 trichlorophene **H41**
 2,3,4-trichlorophenol **T255**
 2,3,5-trichlorophenol **T256**
 2,3,6-trichlorophenol **T257**
 2,4,5-trichlorophenol **T258**
 2,4,6-trichlorophenol **T259**
 3,4,5-trichlorophenol **T260**
 2,4,5-trichlorophenoxyacetic acid **T1**
 2,4,5-trichlorophenoxyacetic acid, butyl ester **B279**
 2-(2,4,5-trichlorophenoxy)ethyl 2,2-dichloropropionate **T261**
 α -(2,4,5-trichlorophenoxy)propionic acid **F14**
 2,3,6-trichlorophenylacetic acid **C124**
 trichlorophenylsilane **P137**
 trichlorophosphine **P166**
 trichlorophosphine oxide **P159**
 trichlorophosphine sulfide **T141**
 1,1,1-trichloropropane **T262**
 1,1,2-trichloropropane **T263**
 1,2,3-trichloropropane **T264**
 1,1,1-trichloropropanone **T227**
 1,1,1-trichloro-2-propanone **T227**
 1,1,3-trichloro-2-propanone **T228**
 1,2,3-trichloro-1-propene **T265**
 3,3,3-trichloro-1-propene **T266**
 S-(2,3,3-trichloro-2-propenyl) bis(1-methylethyl)-carbamothioate **T198**
 trichloro-2-propenylsilane **A94**
 [(3,5,6-trichloro-2-pyridinyl)oxy]acetic acid **T271**
 3,5,6-trichloro-2-pyridyl diethyl phosphorothionate **C313**
 3,5,6-trichloro-2-pyridyloxyacetic acid **T271**
 trichlororhodium **R11**
 trichlorosilane **T267**
 trichlorostibine **A225**
 trichlorotitanium **T167**
 2,4,5-trichlorotoluene **T268**
 α,α,α -trichlorotoluene **B79**
 2,4, 6-trichlorotriazine **C492**
 2,4,6-trichloro-1,3,5-triazine **C492**
 N,N',N''-trichloro-1,3,5-triazine-2,4,6-triamine **T251**
 trichloro-s-triazinetrione **T250**
 1,3,5-trichloro-1,3,5-triazine-2,4,6-(2H,3H,5H)-trione **T250**
 2,2',2''-trichlorotriethylamine **T349**
 1,1,2-trichlorotrifluoroethane **T269**
 1,2,2-trichlorotrifluoroethane **T269**
 trichlorovinylsilane **V39**
 Triclene **T249**
 triclocarban **T270**
 triclopyr **T271**
 Tricodaine **C383**
 tricresol **C456**
 tricresyl phosphate **T361**
 tri-o-cresyl phosphate **T362**
 tricyanogen chloride **C492**
 tricyclazole **T272**
 tricyclazone **T272**
 tricyclo[3.3.1.1^{3,7}]decane **A47**
 1-(tricyclohexylstannyl)-1H-1,2,4-triazole **A270**
 tricyclohexyltin hydroxide **C535**
 tri(cyclohexyl)-1H-1,2,4-triazol-1-yltin **A270**
 Tridal **N209**
 1-tridecanecarboxylic acid **M362**
 1-tridecanol phthalate **D577**
 N-tridecyl-2,6-dimethylmorpholine **T273**

tridemorph **T273**
 tridestrin **O25**
 Tridil **G26**
 2,4,6-tri[(dimethylamino)methyl]phenol **T354**
 tridymite **T274**
 α -tridymite **T274**
 trien **T284**
 trientine **T284**
 trietazine **T275**
 Tri-ethane **T247**
N,N',N''-tri-1,2-ethanediyphosphorothioic triamide **T347**
 triethanolamine **T276**
 triethoxymethane **T286**
 triethoxyphosphine **T288**
 triethoxysilane **T277**
 triethylamine **T278**
 triethyl borate **E101**
 triethyl citrate **T279**
 triethylene glycol **T280**
 triethylene glycol diacrylate **T281**
 triethylene glycol diglycidyl ether **T282**
 triethylene glycol dimethyl ether **T296**
 triethylene glycol monomethyl ether **T283**
 triethylenetetramine **T284**
N,N''-triethylenethiophosphamide **T347**
 triethylenethiophosphoramidate **T347**
 1,3,5-triethylhexahydro-1,3,5-triazine **T285**
 1,3,5-triethylhexahydro-s-triazine **T285**
 triethylhexyl phosphate **T355**
 triethylolamine **T276**
 triethyl orthoformate **T286**
 triethyl phosphate **T287**
 triethyl phosphite **T288**
 triethyltrimethylenetriamine **T285**
 Tri-fen **C124**
 Trifenson **F22**
 5'-[1,1,1-trifluoromethanesulfonamido]acet-2',4'-xylylide **M43**
 triflumizole **T289**
 1,1,1-trifluoroethyl chloride **C300**
 trifluoroacetic acid **T290**
 trifluoroacetic anhydride **T291**
 2,2,2-trifluoroacetic anhydride **T291**
 trifluoroacetyl anhydride **T291**
 trifluoroborane **B147**
 trifluoroboron **B147**
 trifluorobromomethane **B188**
 1,1,1-trifluoro-2-chloroethane **C300**
 2,2,2-trifluorochloroethane **C300**
 trifluorochloroethylene **C301**
 trifluorochloromethane **C302**
 α,α,α -trifluoro-2,6-dinitro-*N,N*-dipropyl-*p*-toluidine **T294**
 trifluoroethanoic acid **T290**
 α,α,α -trifluoro-3'-isopropoxy-*o*-toluanilide **F92**
 trifluoromethane **T292**
 3-(trifluoromethyl)aniline **A118**
 (trifluoromethyl)benzene **B80**
 2-(trifluoromethyl)chlorobenzene **C168**
 3-(trifluoromethyl)chlorobenzene **C169**
 4-(trifluoromethyl)chlorobenzene **C170**
 α,α,α -trifluoro-*N*-methyl-4,6-dinitro-*N*-(2,4,6-tribromophenyl)-*o*-toluidine **B153**
 3-trifluoromethylnitrobenzene **N94**
 4-(trifluoromethyl)nitrobenzene **N95**
m-(trifluoromethyl)nitrobenzene **N94**
 3-(3-trifluoromethylphenyl)-1,1-dimethylurea **F47**
N-(3-trifluoromethylphenyl)-*N,N'*-dimethylurea **F47**
 1,1,1-trifluoro-*N*-[2-methyl-4-(phenylsulfonyl)phenyl]-methanesulfonamide **P54**
 1-(3-trifluoromethyltrityl)-1*H*-1,2,4-triazole **F81**
 trifluoromonobromomethane **B188**
 1,3,5-trifluoro-2-nitrobenzene **T293**
 2,4,6-trifluoronitrobenzene **T293**
 2,2,2-trifluoro-*N*-nitroso-*N*-(2,2,2-trifluoroethyl)ethanamine **N145**
 trifluorostibine **A226**
 α,α,α -trifluorotoluene **B80**
 ω -trifluorotoluene **B80**
 2,4,6-trifluoro-1,3,5-triazine **C493**
 2,2,2-trifluoro-1-(trifluoromethyl)ethanol **H47**
 trifluorovinyl chloride **C301**
 trifluralin **T294**
 Trifolex **M34**
 triforine **T295**
 Triformol **T333**
 Trifungol **F30**
 Trigard **C545**
 Trigen **T280**
 triglyceridase **L51**
 triglycine **N70**
 triglycollamic acid **N70**
 triglycol monomethyl ether **T283**
 triglyme **T296**
 Trigol **T280**
 Trigonox A-80 **B261**
 Trigonox 239A **C475**
 Trigonox C **B271**
 Trigonox 41-C75 **B272**
 Trigonox EHP **D517**
 Trigonox 25-C75 **B273**
 trihexylsilane, *Si*-chloro- **C303**
 1,2,3-trihydroxybenzene **P363**
 trihydroxycyanidine **C491**
 3,4,5-trihydroxy-1-cyclohexene-1-carboxylic acid **S26**
 [3*R*(3 α ,4 α ,5 β)]-3,4,5-trihydroxy-1-cyclohexene-1-carboxylic acid **S26**
 trihydroxyestrin **O25**
 4',5,7-trihydroxyflavanone **N31**
 4',5,7-trihydroxyisoflavone **G9**
 5,7,4'-trihydroxyisoflavone **G9**
 1,3,8-trihydroxy-6-methyl-9,10-anthracenedione **E18**

(1 α ,2 β ,4 α ,4 β ,10 β)-2,4a,7-trihydroxy-1-methyl-8-methyl-ene-gibb-3-ene-1,10-dicarboxylic acid, 1,4a-lactone **G14**
 2 β ,4 α ,7-trihydroxy-1-methyl-8-methylene-4 α ,4 β -gibb-3-ene-1 α ,10 β -dicarboxylic acid 1,4a-lactone **G14**
 trihydroxymethylnitromethane **T357**
 11 β ,17 α ,21-trihydroxypregna-1,4-diene-3,20-dione **P269**
 11,17,21-trihydroxypregn-4-ene-3,20-dione **H95**
 11 β ,17,21-trihydroxyprogesterone **H95**
 trihydroxypropane **G25**
 2,6,8-trihydroxypurine **U14**
 2,4,6-trihydroxy-1,3,5-triazine **C491**
 triiodomethane **I51**
 triisopropanolamine **T297**
 triisopropoxyborane **T298**
 triisopropyl borate **T298**
 triketohydrindene hydrate **N60**
 Triklone **T249**
 trilead phosphate **L27**
 Trilit **T331**
 Trilon B **E8**
 trimanganese tetraoxide **M27**
 Trimangol **M21**
 trimellitic anhydride **T299**
 trimethoprimine **T328**
 2,3,4-trimethacarb **T300**
 3,4,5-trimethacarb **T301**
 trimethanamine **T356**
 trimethoprim **T302**
 trimethoxymethane **T313**
 5-[(3,4,5-trimethoxyphenyl)methyl]-2,4-pyrimidinediamine **T302**
 1,1,1-trimethylacetone **P192**
 trimethylamine **T303**
 1,2,4-trimethyl-5-aminobenzene **T304**
 trimethylaminomethane **B241**
 2,4,5-trimethylaniline **T304**
 2,4,6-trimethylaniline **T305**
 trimethylanilinium chloride **P138**
N,N,N-trimethylanilinium chloride **P138**
 trimethylanilinium iodide **P139**
N,N,N-trimethylanilinium iodide **P139**
 2,4,5-trimethylbenzenamine **T304**
 2,4,6-trimethylbenzenamine **T305**
N,N,N-trimethylbenzenaminiumbenzenaminium iodide **P139**
 1,2,3-trimethylbenzene **T306**
 1,2,4-trimethylbenzene **T307**
 1,2,5-trimethylbenzene **T307**
as-trimethylbenzene **T307**
s-trimethylbenzene **M90**
 trimethylbenzol **M90**
 1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol, acetate **I83**
 1,7,7-trimethylbicyclo[2.2.1]-2-heptanone **C51**
 (1*R*)-2,6,6-trimethylbicyclo[3.1.1]hept-2-ene **P196**
 (1*S*)-2,6,6-trimethylbicyclo[3.1.1]hept-2-ene **P194**
 2,6,6-trimethylbicyclo[3.1.1]hept-2-ene **P195**
 (\pm)-2,6,6-trimethylbicyclo[3.1.1]hept-2-ene **P197**

trimethyl borate **T308**
 trimethylcarbinol **B214**
 β -trimethylchloroethylammonium chloride **C141**
 trimethylchloromethane **B253**
 trimethylchlorosilane **C304**
 trimethylchlorotin **T327**
 1,3,4-trimethylcyclohex-1-ene-4-carboxaldehyde **I100**
 3,5,6-trimethyl-3-cyclohexene-1-carboxaldehyde **I100**
 $\alpha,\alpha,4$ -trimethyl-3-cyclohexene-1-methanol **T36**
 1,1,3-trimethyl-3-cyclohexen-5-one **I110**
 3,5,5-trimethyl-2-cyclohexen-1-one **I110**
 4-(2,6,6-trimethyl-1-cyclohexenyl)-3-buten-2-one **I58**
 3,3,5-trimethylcyclohexylidene bis(*tert*-butyl peroxide) **B117**
 3,3,5-trimethylcyclohexylidene bis(1,1-dimethylethyl peroxide) **B117**
 3,3,5-trimethylcyclohexyl mandelate **C496**
 1,3,7-trimethyl-2,6-dioxopurine **C20**
 trimethylene **C530**
 trimethylene bromochloride **B172**
 trimethylene chlorohydrin **C268**
 trimethylenediamine **D84**
 trimethylene dichloride **D246**
 trimethylene glycol methylene ether **D529**
 trimethylene methylene dioxide **D529**
 trimethylene oxide **T309**
 1,1,1-trimethylethane **N39**
 trimethylethylene **A200**
N,N,N-trimethyl-1-hexadecanaminium bromide **C105**
 trimethylhexadecylammonium bromide **C105**
 trimethyliodomethane **I54**
N,N,N-trimethylmethanaminium hydroxide **T86**
 trimethylmethane **I84**
 1,7,7-trimethylnorcamphor **C50**
 trimethylolaminomethane **T356**
 trimethylolnitromethane **T357**
 trimethylolpropane phosphite **T310**
 trimethylolpropane triacrylate **T311**
 trimethylolpropane trimethacrylate **T312**
 trimethyl orthoformate **T313**
 trimethyl orthophosphate **T324**
 1,3,3-trimethyl-2-oxabicyclo[2.2.2]octane **C343**
 trimethyloxyborane **T308**
 trimethyloxyphosphine **T325**
 2,2,4-trimethylpentane **T314**
 2,2,4-trimethyl-1,3-pentanediol **T315**
 2,2,4-trimethyl-1,3-pentanediol diisobutyrate **T316**
 2,2,4-trimethyl-1,3-pentanediyl diisobutyrate **T316**
 2,4,4-trimethyl-2-pentanethiol **O11**
 2,4,4-trimethylpentene **T317**
 2,4,4-trimethyl-1-pentene **T318**
 2,2,4-trimethylpentyl isobutyrate **T319**
 2,2,4-trimethylpentyl 2-methylpropanoate **T319**
 2,2,4-trimethylpentyl 2-methylpropionate **T319**
*N*⁸,*N*⁸,3-trimethyl-2,8-phenazinediamine monohydrochloride **N42**
 2,3,5-trimethylphenol **T320**

2,3,6-trimethylphenol **T321**
 2,4,6-trimethylphenol **T322**
 3,4,5-trimethylphenol **T323**
 2,3,4-trimethylphenol methylcarbamate **T300**
N,N, α -trimethyl-10*H*-phenothiazine-10-ethanamine **P287**
 trimethylphenylammonium chloride **P138**
 trimethylphenylammonium iodide **P139**
 trimethylphenylmethane **B247**
 3,4,5-trimethylphenylmethylcarbamate **T301**
 trimethyl phosphate **T324**
 trimethyl phosphite **T325**
 trimethylstannyl chloride **T327**
N,N,N-trimethyl-1-tetradecanaminium bromide **M364**
 trimethyltetradecyl ammonium bromide **M364**
 trimethylthiourea **T326**
 trimethyltin chloride **T327**
 1,1,3-trimethyltrimethylenediol **M275**
 1,1,1-trimethyl-*N*-(trimethylsilyl)silanamine **H52**
 2,4,6-trimethyl-1,3,5-trioxane **P9**
 2,4,6-trimethyl-*s*-trioxane **P9**
 1,3,7-trimethylxanthine, 3,7-dihydro-1,3,7-trimethyl-1*H*-
 purine-2,6-dione **C20**
 Trimidal **N209**
 Triminol **N209**
 trimipramine **T328**
 Trimox **A192**
 Trineu **T249**
 trinickel subsulfide **N49**
 trinitrin **G26**
 1,3,5-trinitrobenzene **T329**
s-trinitrobenzene **T329**
 2,4,6-trinitro-1,3-dimethyl-5-*tert*-butyl-benzene **M358**
 2,4,7-trinitrofluorenone **T330**
 2,4,7-trinitro-3*H*-fluoren-9-one **T330**
 trinitroglycerol **G26**
 2,4,6-trinitrophenol **P187**
 2,4,6-trinitrophenol, ammonium salt **A182**
 2,4,6-trinitrophenylmethylnitroamine **N65**
 trinitrotoluene **T331**
 2,4,6-trinitrotoluene **T331**
 α -trinitrotoluol **T331**
 2,4,6-trinitro-*N*-(2,4,6-trinitrophenyl)benzenamine **D550**
 Triocil **H75**
 trioctyl phosphate **T332**
 tri-*n*-octyl phosphate **T332**
 tri-*sec*-octyl phosphate **T355**
 triolein hydrolase **L51**
 3,6,9-trioxadecanol **T283**
 1,3,5-trioxane **T333**
s-trioxane **T333**
 2,5,8-trioxanonane **D338**
 2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane, 4-ethyl-1,3-
 propanediol **T310**
 3,6,9-trioxaundecane **E80**
 2,6,8-trioxopurine **U14**
 trioxychlorofluoride **P53**
 trioxymethylene **T333**
 TRI-PE **D463**
 tripelennamine hydrochloride **T334**
 tri(perfluorobutyl)amine **P55**
 triphenoxyphosphine oxide **T337**
m-triphenyl **T29**
p-triphenyl **T31**
 triphenylamine **T335**
 triphenylchlorostannane **T340**
 triphenylene **T336**
 triphenylmethyl chloride **T363**
 triphenylphosphane **T338**
 triphenyl phosphate **T337**
 triphenyl phosphide **T338**
 triphenylphosphine **T338**
 triphenyl phosphite **T339**
 triphenylphosphorus **T338**
 triphenylsilyl chloride **C305**
 triphenyltin acetate **F25**
 triphenyltin chloride **T340**
 triphenyltin fluoride **T341**
 triphenyltin hydroxide **F26**
 tripropylamine **T342**
 tripropylene **T343**
 tri-*n*-propylene **T343**
 tripropyltin oxide **T344**
 Tripwite **H103**
 trisamine **T356**
 2,3,5-tris(1-aziridinyl)-*p*-benzoquinone **T345**
 2,3,5-tris(1-aziridinyl)-2,5-cyclohexadiene-1,4-dione **T345**
 tris(1-aziridinyl)phosphine oxide **T346**
 tris(1-aziridinyl)phosphine sulfide **T347**
 Tris-BP **T352**
 trisbuffer **T356**
 tris(2-butoxyethanol) phosphate **T348**
 Triscabol **Z19**
 tris(2-chloroethyl)amine **T349**
 tris(β -chloroethyl)amine **T349**
 tris(2-chloroethyl) phosphate **T350**
 tris(β -chloroethyl) phosphate **T350**
 1,2,3-tris(chloromethoxy)propane **T351**
 tris(2,3-dibromopropyl) phosphate **T352**
 tris(1,3-dichloro-2-propyl) phosphate **T353**
 2,4,6-tris(dimethylaminomethyl)phenol **T354**
 tris(dimethylcarbamodithioato-*S,S'*)iron **F30**
 tris(*N,N*-dimethyldithiocarbamato)iron(III) **F30**
 2,4,6-tris(1,1-dimethylethyl)phenol **T211**
 Triserpin **R3**
 tris(2-ethylhexyl) phosphate **T355**
 tris(β -hydroxyethyl)amine **T276**
 1,3,5-tris(2-hydroxyethyl)hexahydro-1,3,5-triazine **H51**
 tris(hydroxymethyl)aminomethane **T356**
 tris(hydroxymethyl)nitromethane **T357**
 tris(2-hydroxypropyl)amine **T297**
 tris(2-methyl-1-aziriny)phosphine oxide **M99**
 tris(*o*-methylphenyl) phosphate **T362**
 tris(nonafluorobutyl)amine **P55**
 trisodiophosphine **S87**

trisodium ethylenediaminetetraacetate trihydrate **E9**
 trisodium nitrilotriacetate, monohydrate **T358**
 trisodium orthophosphate **T359**
 trisodium phosphate **T359**
 trisodium phosphate dodecahydrate **T360**
 trisodium resenate **E9**
 Tri-span **T203**
 tris(2-propenyl) borate **T200**
 1,3,5-tris(2-propenyl)-1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione
T201
 trisulfurated phosphorus **P164**
 Triteren **T203**
 Tritex **A71**
 trithiocarbonic acid, cyclic 2,3-quinoxalinediyl ester
T142
 Trithion **C82**
 tritol **T331**
 tritoyl phosphate **T361**
 tri-*o*-tolyl phosphate **T362**
 Triton TX 100 **O20**
 Triton X100 **O20**
 Tritox **H100**
 Tritox **T229**
 trityl chloride **T363**
 Triumph **I79**
 Triziliu **N112**
 trizinc diphosphide **Z14**
 troclosene **D202**
 Trolene **F8**
 Trometamol **T356**
 Trona Boron Tribromide 99 **B145**
 Tropanol **B245**
 1*αH*,5*αH*-tropan-3*α*-ol (-)-tropate **H124**
 Trophicardyl **I36**
 tropital **P207**
 Tropotox **M34**
 DL-tropyl tropate **A253**
 trotyl **T331**
 Trp-P-1 **T364**
 Trp-P-2 **T365**
 L-Trp **T369**
 Truban **E185**
 Trypan Blue **T366**
 tryptamine **T367**
 tryptophan-P-1 **T364**
 D-tryptophan **T368**
 L-tryptophan **T369**
 tryptophan P2 **T365**
 tryptophol **T370**
 tsiklomitsin **T62**
 TSPP **S88**
 TTZ **M164**
 Tuasol **T208**
 Tuazole **M119**
 Tuberite **P305**
 Tubocin **R15**
 Tubodust **T14**

Tubotin **F26**
 Tuex **T147**
 tungsten **T371**
 tungsten carbide **T372**
 tungsten fluoride **T373**
 tungsten hexafluoride **T373**
 Tunic **M120**
 Turgex **H41**
 turpentine oil **T374**
 turpentine spirit **T374**
 Turplex **A258**
 Tutane **B240**
 Tween 20 **P227**
 Tween 40 **P228**
 Tween 60 **P229**
 Tween 80 **P230**
 tweenase **L51**
 TX 100 **O20**
 Tx60 **V41**
 Tycap **F99**
 Tylical **D316**
 Tylose SL400 **M185**
 tyramine **T375**
 Tyrene **T239**
 tyrosamine **T375**
 Tysul **H103**
 U-6233 **B78**
 U17835 **T170**
 U46 **T1**
 U 6324 **P136**
 UC21149 **A62**
 Ucaricide 225 **G21**
 UDMH **D420**
 Udolac **S146**
 Uifac 6550 **L49**
 Ujoviridin **I30**
 ultracide **M121**
 Ultrafloc **C91**
 Ultra Pure **H87**
 Ultrawet 99LS **S65**
 Umbrathor **T150**
 Unal **A144**
 1,1*a*,2,2*a*,3,3*a*,4,5,5,5*a*,5*b*-undecachlorooctahydro-1,3,4-
 metheno-1*H*-cyclobuta[*cd*]pentalene **P169**
 undecanal **U1**
 undecane **U2**
n-undecane **U2**
 1-undecanethiol **U3**
 undecanoic acid **U4**
 1-undecanol **U5**
 undecan-2-one **U6**
 undecan-6-one **U7**
 2-undecanone **U6**
 6-undecanone **U7**
 undecyl alcohol **U5**
 undecylic acid **U4**
 undecylic aldehyde **U1**

Undene **P315**
 Unichem BZBM **B91**
 Unidigin **D335**
 Unidron **D579**
 Uniflex DOA **D513**
 Unimate DIPA **D357**
 Unimoll BB (BBP) **B94**
 Unimoll 66M (DCHP) **D268**
 Union Carbide Liquid G **S32**
 Uniplex 155 **D354**
 Uniplex 24 **B248**
 Uniplex 250 **D268**
 Uniplex 80 **T279**
 Unislip 1753 **E46**
 Unisom **D599**
 Uniston CR-HT 200 **T159**
 Unisweet SAC **S1**
 Univol U 316S **M362**
 uovocaine **P273**
 Uracil **F79**
 uracil **U8**
 uracil-6-carboxylic acid **O34**
 uracil mustard **B119**
 uracilriboside **U15**
 Uragan **B151**
 Uragan D **H100**
 Uramine T80 **H113**
 uranium **U9**
 uranium-238 **U9**
 uranium, dinitratodioxo **U11**
 uranium nitrate oxide **U11**
 uranium oxyacetate **U10**
 Urantoin **N115**
 uranyl acetate **U10**
 uranyl diacetate **U10**
 uranyl dinitrate **U11**
 uranyl nitrate **U11**
 urea **U12**
 urea, *N,N'*-bis(2-chloroethyl)-*N*-nitroso- **B121**
 urea, 2-bromo-2-ethylbutyryl- **C85**
 urea, 1-[(*p*-chlorophenyl)sulfonyl]-3-propyl- **C311**
 urea, 1-(*o*-chlorophenyl)-2-thio- **C251**
 urea, *N,N'*-diethyl-*N,N'*-diphenyl- **D297**
 urea, *N*-[5-(ethylsulfonyl)-1,3,4-thiadiazol-2-yl]-*N,N'*-dimethyl **E64**
 urea, *N*-methyl-*N'*-(1-methyl-1-phenylethyl)-*N*-phenyl- **M209**
 urea, 1,1,3-trimethyl-2-thio- **T326**
 Ureresolve **E116**
 urethan **U13**
 urethane **U13**
 urethylane **M184**
 Urevert **U12**
 uric acid **U14**
 Uridin **U15**
 uridine **U15**
 Urisal **N4**
 Uritrisin **S141**
 Urlac **C480**
 Urocaudal **T203**
 Urodine **P63**
 Urolong **N115**
 Uroripirin **E16**
 Urox **M351**
 Urox 379 **M351**
 Urox B **B151**
 Urtosal **S5**
 Urushiol **C172**
 USAF A-8565 **G37**
 USAF CF-3 **H30**
 USAF DO-36 **D496**
 USAF EK-1853 **M162**
 USAF EK-2122 **H21**
 USAF EK-3092 **D576**
 USAF EK-4196 **M62**
 USAF EK-4812 **B76**
 USAF EK-6540 **M60**
 USAF EK-7119 **M248**
 USAF EK 1995 **C479**
 USAF GY-3 **M61**
 USAF M-5 **A132**
 USAF P-220 **B74**
 USB3584 **D466**
 Usol Copper Green **C437**
 Ustilan **E64**
 uvic acid **T8**
 Uvinol D-50 **T78**
 Uvinul D-49 **D349**
 UV Titan **T165**
 V17004 **X16**
 Vabrocid **N116**
 VAC **V26**
 Vacor **P362**
 Valamine **I89**
 valeral **V1**
 valeraldehyde **V1**
n-valeraldehyde **V1**
 valerianic acid **V2**
 valerianic aldehyde **V1**
 valeric acid **V2**
 valeric aldehyde **V1**
 δ -valerolactam **P202**
 valerolactone **V3**
 4-valerolactone **V3**
 γ -valerolactone **V3**
 δ -valerosultone **B210**
 D-valine **V4**
 DL-valine **V5**
 L-valine **V6**
 (*R*)-valine **V4**
 (*S*)-valine **V6**
 D-valine cyano(3-phenoxyphenyl)methyl ester **F94**
 valinomycin **V7**
 Valium **D98**

Valkacit LDA **Z9**
 valproic acid **V8**
 Valsan **H103**
 Value SP 20 **S103**
 Valzin **E81**
 Vamidoate **V9**
 vanidothion **V9**
 vanadic acid, ammonium salt **A177**
 vanadic anhydride **V12**
 vanadium **V10**
 vanadium chloride **V13**
 vanadium(III) chloride **V14**
 vanadium(III) oxide **V15**
 vanadium oxysulfate **V16**
 vanadium oxytrichloride **V11**
 vanadium pentoxide **V12**
 vanadium sesquioxide **V15**
 vanadium tetrachloride **V13**
 vanadium trichloride **V14**
 vanadium trioxide **V15**
 vanadyl sulfate **V16**
 vanadyl trichloride **V11**
 Vanax DPG **D545**
 Vancide **T285**
 Vancide BL **T122**
 Vancide BN **S49**
 Vancide P **Z15**
 Vandex **S14**
 Vanicol **S112**
 vanilla **V17**
 vanillaldehyde **V17**
 vanillic aldehyde **V17**
 vanillin **V17**
 p-vanillin **V17**
 Vanox 12 **D516**
 Vanox ODP **D516**
 Vanox PCX **B245**
 Vansil **C43**
 Vapam **M96**
 Varisoft 250 **C105**
 Varitox **S97**
 varnoline **S119**
 Vasal **P5**
 Vasolklin **T155**
 Vasoperif **C60**
 Vat Blue 1 **I25**
 VC25074 **F106**
 VCR **V24**
 VCR sulfate **V25**
 VDF **D332**
 Vegadex **S135**
 vegetable pepsin **P3**
 VEL 3973 **M43**
 Velardon **P3**
 Velban **V21**
 Velbe **V21**
 Velflon **P232**

Velpar **H69**
 Vendex **F7**
 Venetian red **I74**
 Vengeance **B153**
 Veracin **T62**
 veratric acid, 4-[ethyl(p-methoxy- α -methylphenethyl)-amino]butyl ester **M35**
 veratrole **V18**
 Verazinc white copperas **Z17**
 Verdasan **E40**
 Verdet **C430**
 Verisan **I62**
 Vernam **V19**
 vernolate **V19**
 versene acid **E3**
 Versene AG **E5**
 Vertolan **S133**
 Vestamin IPD **I111**
 Vestanat IPDI **I112**
 Vestinol AH **D519**
 Vestolit **P235**
 Vetrazin **C545**
 Vibalt **C368**
 Vi-Cad **C5**
 vicknite **P257**
 Victenon **B37**
 Victoria Scarlet 3R **C394**
 Vienna Green **P15**
 Vigor **L34**
 Vikane **S158**
 Vinadine **O55**
 Vinamar **E181**
 Vinarol **P234**
 vinblastine **V20**
 vinblastine sulfate **V21**
 vinburnine **V22**
 vincalcucoblastine sulfate **V21**
 Vincalcucoblastine **V20**
 vincalcucoblastine sulfate (1:1) **V21**
 vincamone **V22**
 vinclozolin **V23**
 vincristine **V24**
 vincristine sulfate **V25**
 Vincrisul **V25**
 vinegar acid **A12**
 vinegar naphtha **E87**
 vinethene **D581**
 Vinicur **C544**
 vinyl acetate **V26**
 vinyl acetate homopolymer **P233**
 vinyl acetate resin **P233**
 vinyl alcohol **V27**
 vinyl alcohol polymer **P234**
 vinyl A monomer **V26**
 vinylbenzene **S126**
 vinylbenzol **S126**
 vinyl bromide **V28**

vinyl butyl ether **B280**
 vinylbutylolactam **V37**
 vinyl butyrate **V29**
 vinyl carbinol **A73**
 vinyl carbonyl butyrate **A77**
 vinyl carbonylcinnamate **A80**
 vinyl chloride **V30**
 vinyl chloride homopolymer **P235**
 vinyl chloride monomer **V30**
 vinyl 2-chloroethyl ether **C199**
 vinyl β -chloroethyl ether **C199**
 vinyl cyanide **A43**
 1-vinylcyclohex-3-ene **V31**
 4-vinyl-1-cyclohexene **V31**
 (\pm)-4-vinyl-1-cyclohexene diepoxide **V32**
 4-vinylcyclohexene dioxide **V32**
 vinyl ether **D581**
 vinylethylene **B197**
 vinyl ethyl ether **E181**
 vinyl fluoride **V33**
 vinylformic acid **A42**
 vinylidene chloride **D212**
 vinylidene difluoride **D332**
 vinylidene fluoride **D332**
 vinyl isobutyl ether **I96**
 vinyl methyl ether **M317**
 2-vinylbornene **V34**
 5-vinyl-2-norbornene **V34**
 2-vinylloxyethyl chloride **V299**
 5-vinyl-2-picoline **M319**
 2-vinylpyridine **V35**
 4-vinylpyridine **V36**
 1-vinyl-2-pyrrolidinone **V37**
 N-vinylpyrrolidinone **V37**
 N-vinyl-2-pyrrolidinone **V37**
 1-vinyl-2-pyrrolidinone polymers **P236**
 vinylsilicon trichloride **V39**
 vinylstyrene **D580**
 vinyl sulfone **V38**
 vinyltoluene (mixed isomers) **M306**
 vinyl trichloride **T248**
 vinyltrichlorosilane **V39**
 Vinyzene **O55**
 violaquercetin **R22**
 violet 3 **X8**
 Virem **V23**
 Virexan **I48**
 virosterone **T38**
 Viscarin **C91**
 visosal **M185**
 Visumetazone **D62**
 vitamin A **V40**
 13-*cis*-vitamin A acid **I138**
 vitamin A (all-*trans*) **R7**
 vitamin B₁ **T113**
 vitamin B₁ **T112**
 vitamin B₁₂ **C368**
 vitamin B₂ **R12**
 vitamin B₆ **P358**
 Vitamin B₇ **B112**
 vitamin B_c **F96**
 Vitamin B_x **A117**
 vitamin B₆ hydrochloride **P359**
 vitamin C **A248**
 vitamin D₂ **E42**
 vitamin D₃ **C323**
 vitamin E **T169**
 vitamin G **R12**
 Vitamin H **B112**
 vitamin K₁ **P181**
 Vitamin L **A115**
 vitamin M **F96**
 vitamin PP **N53**
 Vitavax **C84**
 Vitavax sulfone **O56**
 viticosterone **E1**
 vitreous silica **S29**
 vitriol brown oil **S152**
 VLB **V20**
 VLB sulfate **V21**
 Vogan **R7**
 Volaton **P170**
 Volfazol **M167**
 Vorlan **V23**
 Voronit **F113**
 Votexit **T225**
 VP 19-40 **F25**
 4-VP **V36**
 V-Pyrol **V37**
 VSAF GY-7 **Z10**
 VT 1-1 **T164**
 Vulcalent A **N155**
 Vulcanox HS/LG **A16**
 Vulkacit ZM **Z10**
 Vulkanox PBN **P124**
 Vulklor **C115**
 Vultrol **N155**
 Vulvic acid **L8**
 VX **V41**
 VX Vapour **V41**
 VYAC **V26**
 Vydate **O47**
 Vynamon Blue A **I25**
 W 524 **T295**
 Walkerde Flygtol GA **M349**
 Waloran N **C98**
 Warbex **F1**
 Warcoumin **W3**
 warfarin **W1**
 (+)-warfarin **W2**
 (\pm)-warfarin **W1**
 R-(+)-warfarin **W2**
 warfarin sodium **W3**
 Warfilone **W3**

Water Red 2 **E29**
 wattle gum **G53**
 WC-Reiniger **P156**
 Weedazol **A160**
 Weed Ender **C1**
 Wepsin **T202**
 Westron **T50**
 W-Gum **S110**
 whey factor **O34**
 Whip **F16**
 white arsenic **A244**
 white spirit **S119**
 white tar **N9**
 White vitriol **Z17**
 Wijs' chloride **I41**
 Willbutamide **T171**
 Wilpo **P88**
 Win 20228 **P42**
 wintergreen oil **M305**
 Wintomylon **N4**
 Wipeout **H86**
 Witconate 605A **C32**
 Witox **E40**
 Wizzard **F39**
 WL2236 **F10**
 WM 842 **B138**
 Wofaverdin **I30**
 wood alcohol **M116**
 wood ether **D413**
 wood naphtha **M116**
 wood spirit **M116**
 wood sugar **X14**
 Wool Green S **C389**
 Wool Violet 4BN **B101**
 Worm-away **P200**
 wormwood acid **S128**
 WP 155 **T202**
 Wurmiazin **P200**
 Wurster's blue **T92**
 Wurster's reagent **T92**
 WV 90043a **C536**
 Wy-401 **E73**
 Wytox LT **D365**
 Xan **X2**
 xanthaurine **Q2**
 xanthene **X1**
 9H-xanthene **X1**
 xanthenone **X3**
 9-xanthenone **X3**
 9H-xanthen-9-one **X3**
 Xanthic oxide **X2**
 xanthine **X2**
 xanthone **X3**
 Xanthotoxin **M129**
 Xedamine **D540**
 o-xenol **P125**
 xenylamine **A121**
 XL All Insecticide **N54**
 XMC **X4**
 3,5-XMC **X4**
 XOE 2982 **H29**
 xydiphone **E183**
 1,2-xylene **X6**
 1,3-xylene **X5**
 1,4-xylene **X7**
 m-xylene **X5**
 o-xylene **X6**
 p-xylene **X7**
 m-xylene- α,α' -diamine **X17**
 p-xylene, α,α' -dimethyl- **D294**
 xylene (mixed isomers) **X8**
 xylenol **X9**
 1,2,5-xylenol **X11**
 1,3,5-xylenol **X12**
 2,4-xylenol **X10**
 2,5-xylenol **X11**
 3,5-xylenol **X12**
 m-xylenol **X10**
 p-xylenol **X11**
 sym-m-xylenol **X12**
 3,5-xylenyl N-methylcarbamate **X4**
 Xylidene Ponceau 2R **C395**
 2,3-xylidine **D395**
 2,4-xylidine **D396**
 2,5-xylidine **D397**
 2,6-xylidine **D398**
 3,4-xylidine **D399**
 3,5-xylidine **D400**
 m-xylidine **D396**
 o-xylidine **D398**
 o-xylidine **D395**
 p-xylidine **D397**
 Xylene **L43**
 xylit **X13**
 xylitol **X13**
 meso-xylitol **X13**
 Xylocitin **L43**
 xylol **X8**
 m-xylol **X5**
 o-xylol **X6**
 p-xylol **X7**
 xylomed **X14**
 Xylo-Pfan **X14**
 (+)-xylose **X14**
 D-xylose **X14**
 L-xylose **X15**
 2,3-xylylamine **D395**
 2,4-xylylamine **D396**
 2,6-xylylamine **D398**
 3,4-xylylamine **D399**
 3,5-xylylamine **D400**
 N-2,3-xylylanthranilic acid **M42**
 1-(2,4-xylylazo)-2-naphthol **C420**
 1-(m-xylylazo)-2-naphthol **C420**

xylylcarb **X16**
m-xylylenediamine **X17**
o-xylylene sulfide **D343**
 3,4-xylyl methylcarbamate **X16**
 3,5-xylyl methylcarbamate **X4**
 Yamamoto Methylene Blue ZF **M216**
 Yanock **F53**
 Yardex **F94**
 Yeer **B196**
 yellow mercury iodide **M75**
 yellow ultramarine **C28**
 yohimban-16-carboxylic acid, 11,17-dimethoxy-18-[(3,4,5-trimethoxybenzoyl)oxy]-, methyl ester, (3 β ,16 β ,17 α ,18 β ,20 α)- **R3**
 yohimbic acid methyl ester **Y1**
 (+)-yohimbine **Y1**
 Yomesan **N52**
 Yoshi 864 **I16**
 yperite **M359**
 yttrium **Y2**
 yttrium chloride **Y3**
 yttrium nitrate **Y4**
 yttrium (3+) nitrate **Y4**
 yttrium(III) nitrate **Y4**
 yttrium trichloride **Y3**
 yttrium trinitrate **Y4**
 Zactane **E73**
 Zadoary oil **C343**
 Zaprawa Marshal **C83**
 Zaron **B137**
 Z-cote **Z12**
 Zean **E40**
 zearalenone **Z1**
 (-)-zearalenone **Z1**
 (s)-zearalenone **Z1**
trans-zearalenone **Z1**
 Zectran **M331**
 Zeldox **H80**
 Zellek **H5**
 Zenite **Z10**
 Zepelin **F29**
 Zertell **C314**
 Zeset T **V26**
 Ziarnik **P116**
 zimanat **M19**
 Zimco **V17**
 Zinamide **P348**
 zinc **Z2**
 zinc acetate **Z3**
 zinc ammoniate ethylenebis(dithiocarbamate)-poly(ethyleneethiuram disulfide) **M321**
 zinc benzenesulfonate **Z13**
 zinc-2-benzothiazolethiolate **Z10**
 zinc bis(dimethyldithiocarbamate) **Z19**
 zinc bromide **Z4**
 zinc carbonate **Z5**
 zinc chloride **Z6**
 zinc chloride 3-chloro-4-diethylaminobenzenediazonium chloride (1:1) complex **C190**
 zinc chromate **Z7**
 zinc chromate(VI) hydroxide **Z7**
 zinc chrome yellow **Z7**
 zinc chromium yellow **Z7**
 zinc cyanide **Z8**
 zinc diacetate **Z3**
 zinc dibromide **Z4**
 zinc dichloride **Z6**
 zinc dicyanide **Z8**
 zinc diethyldithiocarbamate **Z9**
 zinc *N,N*-diethyldithiocarbamate **Z9**
 zinc *N,N*-dimethyldithiocarbamate **Z19**
 zinc dinitrate **Z11**
 zinc distearate **Z16**
 zinc ethylenebis(dithiocarbamate) (polymeric) **Z18**
 zinc hydroxychromate **Z7**
 zinc 2-mercaptobenzothiazole **Z10**
 zinc, [[(1-methyl-1,2-ethanediy)bis(carbamodithioato)](2-)]- **P307**
 zinc muriate **Z6**
 zinc nitrate **Z11**
 zinc octadecanoate **Z16**
 zinc omadine **Z15**
 zinc oxide **Z12**
 zinc *p*-phenolsulfonate **Z13**
 zinc phosphide **Z14**
 zinc polyanemine **Z15**
 zinc 1,2-propylene bisdithiocarbamate **P307**
 zinc, [propylenebis (dithiocarbamato)]- **P307**
 zinc PT **Z15**
 zinc pyridinethione **Z15**
 zinc pyrron **Z15**
 zinc pyrithione **Z15**
 zinc stearate **Z16**
 zinc sulfate **Z17**
 zinc sulfocarbolate **Z13**
 Zinc-Tox **Z14**
 zinc vitriol **Z17**
 zineb **Z18**
 Zinespar **Z5**
 Zinophos **T135**
 Zinox **Z12**
 ziram **Z19**
 zirconyl sulfate **Z23**
 zirconate(2-), hexafluoro-, dipotassium (OC-6-11)- **P251**
 zirconium **Z20**
 zirconium chloride **Z24**
 zirconium(IV) chloride **Z24**
 zirconium dihydride **Z21**
 zirconium hydride **Z21**
 zirconium nitrate **Z22**
 zirconium potassium fluoride **P251**
 zirconium sulfate **Z23**
 zirconium(IV) sulfate **Z23**
 zirconium tetrachloride **Z24**

zirconium tetranitrate **Z22**
Zoaline **D465**
Zobar **T10**
Zolone **P149**
Zoocoumarin **W1**
Zoofurin **N115**
Zorane **N207**
Zorial **N206**

zoxamin **Z25**
zoxazolamine **Z25**
ZP **Z14**
ZPT **Z15**
Zyloprim **A70**
Zyloric **A70**
ZZ-Doricide **B37**

Index of CAS Registry Numbers

50-00-0	formaldehyde F100	51-79-6	urethane U13
50-01-1	guanidine hydrochloride G48	51-83-2	carbachol chloride C60
50-02-2	dexamethasone D62	52-01-7	spironolactone S108
50-06-6	phenobarbitone P79	52-24-4	tris(1-aziridiny)phosphine sulfide T347
50-07-7	mitomycin M336	52-28-8	codeine phosphate C383
50-14-6	ergocalciferol E42	52-46-0	apholate A229
50-18-0	cyclophosphamide C529	52-51-7	bronopol B190
50-21-5	lactic acid L1	52-68-6	trichlorfon T225
50-23-7	hydrocortisone H95	52-76-6	lynestrenol L67
50-24-8	prednisolone P269	52-85-7	famphur F1
50-27-1	oestriol O25	53-16-7	estrone E53
50-28-2	estradiol E50	53-19-0	<i>o,p'</i> -DDD D29
50-29-3	<i>p,p'</i> -DDT D35	53-60-1	promazine hydrochloride P285
50-30-6	2,6-dichlorobenzoic acid D194	53-70-3	dibenz[<i>a,h</i>]anthracene D103
50-31-7	2,3,6-TBA T10	53-86-1	indomethacin I35
50-32-8	benzo[<i>a</i>]pyrene B71	53-95-2	<i>N</i> -hydroxy-2-acetylaminofluorene H109
50-33-9	phenylbutazone P96	53-96-3	2-acetylaminofluorene A23
50-35-1	thalidomide T99	54-05-7	chloroquine C281
50-41-9	clomiphene citrate C361	54-11-5	nicotine N54
50-44-2	6-mercaptopurine M63	54-31-9	frusemide F112
50-48-6	amitriptyline A159	54-32-0	thymoxamine T155
50-49-7	imipramine I14	54-36-4	metyrapone M329
50-52-2	thioridazine T143	54-42-2	5-iodo-2'-deoxyuridine I48
50-53-3	chlorpromazine C310	54-62-6	aminopterin A150
50-55-5	reserpine R3	54-64-8	thiomersal T133
50-65-7	niclosamide N52	54-71-7	pilocarpine hydrochloride P190
50-70-4	D-sorbitol S104	54-85-3	isoniazid I109
50-76-0	actinomycin D A46	55-18-5	<i>N</i> -nitrosodiethylamine N149
50-78-2	acetylsalicylic acid A28	55-21-0	benzamide B42
50-81-7	ascorbic acid A248	55-38-9	fenthion F24
50-99-7	D-glucose G17	55-56-1	chlorhexidine C130
51-03-6	piperonyl butoxide P204	55-63-0	glycerol trinitrate G26
51-12-7	nialamide N43	55-91-4	isofluorophate I106
51-17-2	benzimidazole B53	55-98-1	busulfan B195
51-21-8	5-fluorouracil F79	56-04-2	6-methyl-2-thiouracil M312
51-28-5	2,4-dinitrophenol D486	56-18-8	norspermidine N208
51-34-3	hyoscyne H122	56-23-5	carbon tetrachloride C78
51-43-4	L-adrenaline A51	56-25-7	cantharidin C54
51-44-5	3,4-dichlorobenzoic acid D195	56-29-1	hexobarbital H76
51-48-9	L-thyroxine T156	56-35-9	tributyltin oxide T219
51-52-5	6-propyl-2-thiouracil P337	56-36-0	tributyltin acetate T213
51-55-8	atropine A253	56-38-2	parathion P13
51-61-6	dopamine D595	56-40-6	glycine G36
51-67-2	tyrosamine T375	56-49-5	3-methylcholanthrene M190
51-75-2	mechlorethamine M38	56-53-1	stilbestrol S116

56-55-3	benz[a]anthracene	B43	58-96-8	uridine	U15
56-72-4	coumaphos	C446	59-02-9	α -tocopherol	T169
56-75-7	chloramphenicol	C114	59-05-2	methotrexate	M128
56-81-5	glycerol	G25	59-30-3	folic acid	F96
56-82-6	glyceraldehyde	G23	59-31-4	2-hydroxyquinoline	H118
57-06-7	allyl isothiocyanate	A87	59-42-7	phenylephrine	P106
57-09-0	cetyltrimethylammonium bromide	C105	59-43-8	thiamine	T112
57-11-4	stearic acid	S112	59-46-1	procaine	P273
57-12-5	cyanide	C481	59-50-7	4-chloro- <i>m</i> -cresol	C183
57-13-6	urea	U12	59-52-9	dimercaprol	D369
57-14-7	1,1-dimethylhydrazine	D420	59-67-6	nicotinic acid	N57
57-22-7	vincristine	V24	59-87-0	nitrofurazone	N116
57-24-9	strychnine	S125	59-88-1	phenylhydrazine hydrochloride	P109
57-27-2	morphine	M352	59-89-2	<i>N</i> -nitrosomorpholine	N166
57-39-6	metepa	M99	59-92-7	levodopa	L37
57-41-0	phenytoin	P141	60-00-4	EDTA	E3
57-43-2	amylobarbitone	A204	60-01-5	tributyrin	T223
57-47-6	physostigmine	P178	60-09-3	4-aminoazobenzene	A114
57-48-7	D-fructose	F111	60-10-6	dithizone	D576
57-50-1	sucrose	S131	60-11-7	Methyl Yellow	M320
57-53-4	meprobamate	M57	60-12-8	phenethyl alcohol	P67
57-55-6	propylene glycol	P327	60-24-2	2-mercaptoethanol	M62
57-57-8	β -propiolactone	P308	60-29-7	diethyl ether	D304
57-62-5	7-chlortetracycline	C316	60-33-3	linoleic acid	L49
57-63-6	ethinyloestradiol	E66	60-34-4	methylhydrazine	M234
57-64-7	physostigmine salicylate	P179	60-35-5	acetamide	A10
57-67-0	sulfaguanidine	S134	60-51-5	dimethoate	D376
57-68-1	sulfadimidine	S133	60-54-8	tetracycline	T62
57-74-9	chlordanes	C118	60-56-0	methimazole	M122
57-83-0	progesterone	P282	60-57-1	dieldrin	D276
57-87-4	ergosterol	E43	60-87-7	promethazine	P287
57-88-5	cholesterol	C324	61-25-6	papaverine hydrochloride	P5
57-91-0	α -estradiol	E51	61-33-6	benzylpenicillin	B100
57-97-6	7,12-dimethylbenz[a]anthracene	D401	61-54-1	tryptamine	T367
58-08-2	caffeine	C20	61-57-4	niridazole	N62
58-14-0	pyrimethamine	P361	61-68-7	mefenamic acid	M42
58-15-1	aminopyrine	A154	61-73-4	Methylene Blue	M216
58-22-0	testosterone	T38	61-80-3	zoxazolamine	Z25
58-25-3	chlordiazepoxide	C120	61-82-5	amitrole	A160
58-36-6	10,10'-oxybisphenoxarsine	O55	62-23-7	4-nitrobenzoic acid	N89
58-38-8	prochlorperazine	P276	62-33-9	EDTA calcium disodium salt	E4
58-55-9	theophylline	T110	62-38-4	phenylmercuric acetate	P116
58-56-0	pyridoxine hydrochloride	P359	62-44-2	phenacetin	P58
58-63-9	inosine	I36	62-49-7	choline	C326
58-73-1	diphenhydramine	D537	62-50-0	ethyl methanesulfonate	E146
58-74-2	papaverine	P4	62-53-3	aniline	A209
58-85-5	biotin	B112	62-55-5	thioacetamide	T115
58-86-6	D-xylose	X14	62-56-6	thiourea	T146
58-89-9	γ -HCH	H10	62-73-7	dichlorvos	D258
58-90-2	2,3,4,6-tetrachlorophenol	T55	62-74-8	sodium fluoroacetate	S67
58-93-5	hydrochlorothiazide	H94	62-75-9	dimethylnitrosamine	D444
58-94-6	chlorothiazide	C287	63-25-2	carbaryl	C63

63-91-2	L-phenylalanine	P92	68-96-2	hydroxyprogesterone	H115
63-92-3	phenoxybenzamine hydrochloride	P85	69-53-4	ampicillin	A194
64-00-6	3-isopropylphenyl methylcarbamate	I131	69-65-8	D-mannitol	M28
64-02-8	EDTA tetrasodium salt	E8	69-72-7	salicylic acid	S6
64-04-0	phenethylamine	P69	69-89-6	xanthine	X2
64-17-5	ethanol	E61	69-93-2	uric acid	U14
64-18-6	formic acid	F104	70-22-4	oxotremorin	O51
64-19-7	acetic acid	A12	70-25-7	1-methyl-3-nitro-1-nitrosoguanidine	M265
64-67-5	diethyl sulfate	D317	70-30-4	hexachlorophene	H41
64-69-7	iodoacetic acid	I42	70-34-8	2,4-dinitrofluorobenzene	D476
64-73-3	demeclocycline hydrochloride	D48	70-55-3	<i>p</i> -toluenesulfonamide	T178
64-77-7	tolbutamide	T171	70-69-9	4'-aminopropiophenone	A149
64-86-8	colchicine	C384	71-23-8	1-propanol	P296
65-23-6	pyridoxine	P358	71-36-3	1-butanol	B212
65-30-5	nicotine sulfate	N55	71-41-0	1-pentanol	P41
65-31-6	nicotine tartrate	N56	71-43-2	benzene	B47
65-45-2	salicylamide	S5	71-44-3	spermine	S107
65-71-4	thymine	T153	71-55-6	1,1,1-trichloroethane	T247
65-85-0	benzoic acid	B63	71-63-6	digitoxin	D335
65-86-1	orotic acid	O34	72-18-4	L-valine	V6
66-22-8	uracil	U8	72-19-5	L-threonine	T152
66-25-1	hexanal	H59	72-20-8	endrin	E25
66-27-3	methyl methanesulfonate	M253	72-33-3	mestranol	M92
66-56-8	2,3-dinitrophenol	D485	72-43-5	methoxychlor	M132
66-71-7	1,10-phenanthroline	P60	72-44-6	methaqualone	M119
66-75-1	5-bis(2-chloroethyl)aminouracil	B119	72-54-8	<i>p,p'</i> -DDD	D30
66-76-2	dicoumarin	D262	72-55-9	<i>p,p'</i> -DDE	D31
66-77-3	1-naphthaldehyde	N7	72-56-0	1,1-dichloro-2,2-bis(4-ethylphenyl)ethane	D199
66-81-9	cycloheximide	C513		Trypan Blue	T366
66-86-4	neomycin C	N37	72-57-1	L-tryptophan	T369
66-97-7	psoralen	P344	73-22-3	melatonin	M48
66-99-9	2-naphthaldehyde	N8	73-31-4	guanine	G50
67-03-8	thiamine hydrochloride	T113	73-40-5	methane	M112
67-20-9	nitrofurantoin	N115	74-82-8	bromomethane	B178
67-45-8	furazolidone	F126	74-83-9	ethane	E58
67-56-1	methanol	M116	74-84-0	ethylene	E113
67-63-0	2-propanol	P297	74-85-1	acetylene	A26
67-64-1	acetone	A17	74-86-2	chloromethane	C206
67-66-3	chloroform	C201	74-87-3	iodomethane	I52
67-68-5	dimethyl sulfoxide	D458	74-88-4	methylamine	M154
67-71-0	dimethyl sulfone	D457	74-89-5	hydrogen cyanide	H100
67-72-1	hexachloroethane	H38	74-90-8	methanethiol	M115
67-97-0	cholecalciferol	C323	74-93-1	dibromomethane	D133
68-11-1	mercaptoacetic acid	M59	74-95-3	bromoethane	B175
68-12-2	dimethylformamide	D416	74-96-4	bromochloromethane	B171
68-19-9	cobalamin	C368	74-97-5	propane	P292
68-22-4	norethisterone	N204	74-98-6	propyne	P338
68-23-5	norethynodrel	N205	74-99-7	chloroethane	C196
68-26-8	retinol	R7	75-00-3	vinyl chloride	V30
68-35-9	sulfadiazine	S132	75-01-4	vinyl fluoride	V33
68-76-8	2,3,5-tris(1-aziridinyl)- <i>p</i> -benzoquinone	T345	75-02-5	iodoethane	I49
			75-03-6		

75-04-7	ethylamine E90	75-88-7	2-chloro-1,1,1-trifluoroethane C300
75-05-8	acetonitrile A20	75-91-2	<i>tert</i> -butyl hydroperoxide B261
75-07-0	acetaldehyde A7	75-94-5	vinyltrichlorosilane V39
75-08-1	ethanethiol E60	75-97-8	pinacolone P192
75-09-2	dichloromethane D222	75-99-0	dalapon D19
75-12-7	formamide F101	76-01-7	pentachloroethane P28
75-15-0	carbon disulfide C75	76-02-8	trichloroacetyl chloride T230
75-18-3	dimethyl sulfide D456	76-03-9	trichloroacetic acid T226
75-19-4	cyclopropane C530	76-05-1	trifluoroacetic acid T290
75-20-7	calcium carbide C24	76-06-2	chloropicrin C259
75-21-8	ethylene oxide E120	76-11-9	1,1-difluorotetrachloroethane D333
75-25-2	bromoform B177	76-12-0	1,2-difluorotetrachloroethane D334
75-26-3	2-bromopropane B186	76-13-1	1,1,2-trichlorotrifluoroethane T269
75-27-4	bromodichloromethane B173	76-14-2	1,2-dichlorotetrafluoroethane D252
75-28-5	isobutane I84	76-15-3	chloropentafluoroethane C234
75-29-6	2-chloropropane C264	76-16-4	hexafluoroethane H46
75-31-0	isopropylamine I121	76-19-7	octafluoropropane O7
75-34-3	1,1-dichloroethane D210	76-22-2	camphor C50
75-35-4	1,1-dichloroethylene D212	76-38-0	methoxyfluorane M138
75-36-5	acetyl chloride A25	76-44-8	heptachlor H15
75-37-6	1,1-difluoroethane D330	76-58-4	ethylmorphine E151
75-38-7	1,1-difluoroethylene D332	76-73-3	quinalbarbitone Q3
75-43-4	dichlorofluoromethane D216	76-74-4	pentobarbitone P45
75-44-5	phosgene P152	76-83-5	trityl chloride T363
75-45-6	chlorodifluoromethane C192	76-86-8	chlorotriphenylsilane C305
75-46-7	trifluoromethane T292	76-87-9	fentin hydroxide F26
75-47-8	iodoform I51	77-06-5	gibberellic acid G14
75-50-3	trimethylamine T303	77-09-8	phenolphthalein P81
75-52-5	nitromethane N127	77-15-6	ethoheptazine E73
75-54-7	dichloromethylsilane D225	77-21-4	glutethimide G22
75-55-8	2-methylaziridine M158	77-28-1	butobarbitone B222
75-56-9	propylene oxide P330	77-36-1	chlorthalidone C318
75-59-2	tetramethylammonium hydroxide T86	77-47-4	hexachlorocyclopentadiene H35
75-60-5	cacodylic acid C1	77-58-7	dibutyltin dilaurate D163
75-61-6	dibromodifluoromethane D131	77-65-6	carbromal C85
75-63-8	bromotrifluoromethane B188	77-73-6	dicyclopentadiene D271
75-64-9	<i>tert</i> -butylamine B241	77-74-7	3-methyl-3-pentanol M279
75-65-0	<i>tert</i> -butanol B214	77-77-0	vinyl sulfone V38
75-68-3	1-chloro-1,1-difluoroethane C191	77-78-1	dimethyl sulfate D455
75-69-4	fluorotrichloromethane F78	77-79-2	3-sulfolene S144
75-71-8	dichlorodifluoromethane D204	77-81-6	Tabun T2
75-72-9	chlorotrifluoromethane C302	77-86-1	tris(hydroxymethyl)aminomethane T356
75-73-0	carbon tetrafluoride C79	77-92-9	citric acid C352
75-74-1	tetramethyllead T90	77-93-0	triethyl citrate T279
75-75-2	methanesulfonic acid M113	78-00-2	tetraethyllead T66
75-76-3	tetramethylsilane T93	78-10-4	tetraethyl orthosilicate T67
75-77-4	chlorotrimethylsilane C304	78-18-2	cyclohexanone hydroperoxide C510
75-78-5	dichlorodimethylsilane D206	78-30-8	tri- <i>o</i> -tolyl phosphate T362
75-79-6	methyltrichlorosilane M314	78-34-2	dioxathion D531
75-85-4	2-methyl-2-butanol M173	78-40-0	triethyl phosphate T287
75-86-5	acetone cyanohydrin A18	78-42-2	tris(2-ethylhexyl) phosphate T355
75-87-6	chloral C107	78-48-8	tribufos T209

78-51-3	tris(2-butoxyethanol) phosphate T348	79-43-6	dichloroacetic acid D172
78-53-5	amiton A156	79-44-7	dimethylcarbamyl chloride D406
78-57-9	menazon M50	79-46-9	2-nitropropane N139
78-59-1	isophorone I110	79-57-2	oxytetracycline O64
78-62-6	diethoxydimethylsilane D284	79-77-6	β -ionone I58
78-67-1	azobis(isobutyronitrile) A269	79-92-5	camphene C49
78-70-6	linalool L47	79-94-7	tetrabromobisphenol A T39
78-71-7	3,3-bis(chloromethyl)oxetane B124	80-05-7	bisphenol A B133
78-76-2	2-bromobutane B165	80-06-8	chlorfenethol C125
78-78-4	2-methylbutane M172	80-07-9	bis(4-chlorophenyl) sulfone B127
78-79-5	isoprene I115	80-08-0	4,4'-sulfonyldianiline S146
78-81-9	isobutylamine I89	80-10-4	dichlorodiphenylsilane D209
78-82-0	isobutyronitrile I99	80-11-5	<i>N</i> -methyl- <i>N</i> -nitroso- <i>p</i> -toluenesulfonamide M269
78-83-1	isobutanol I85		
78-84-2	isobutyraldehyde I97	80-15-9	cumene hydroperoxide C475
78-85-3	methacrolein M103	80-17-1	benzenesulfonyl hydrazide B49
78-86-4	<i>sec</i> -butyl chloride B252	80-33-1	chlorfenson C127
78-87-5	1,2-dichloropropane D245	80-38-6	fenson F22
78-88-6	2,3-dichloropropene D251	80-40-0	ethyl <i>p</i> -toluenesulfonate E179
78-89-7	2-chloropropanol C267	80-43-3	dicumyl peroxide D264
78-90-0	1,2-diaminopropane D83	80-46-6	4- <i>tert</i> -amylphenol A205
78-92-2	2-butanol B213	80-48-8	methyl <i>p</i> -toluenesulfonate M313
78-93-3	methyl ethyl ketone M220	80-51-3	4,4'-oxybis(benzenesulfonyl hydrazide) O53
78-94-4	methyl vinyl ketone M318		
78-95-5	chloroacetone C146	80-53-5	terpin T32
78-96-6	1-amino-2-propanol A148	80-54-6	lilial L44
78-97-7	lactonitrile L2	80-56-8	α -pinene P195
78-99-9	1,1-dichloropropane D244	80-59-1	tiglic acid T157
79-00-5	1,1,2-trichloroethane T248	80-62-6	methyl methacrylate M252
79-01-6	trichloroethylene T249	80-63-7	methyl 2-chloroacrylate M187
79-03-8	propionyl chloride P313	80-71-7	maple lactone M31
79-04-9	chloroacetyl chloride C151	80-82-0	2-nitrobenzenesulfonic acid N83
79-06-1	acrylamide A41	81-07-2	saccharin S1
79-07-2	2-chloroacetamide C144	81-11-8	4,4'-diamino-2,2'-stilbenedisulfonic acid D85
79-08-3	bromoacetic acid B158		
79-09-4	propionic acid P310	81-15-2	musk xylene M358
79-10-7	acrylic acid A42	81-16-3	2-aminonaphthalene-1-sulfonic acid A131
79-11-8	chloroacetic acid C145	81-20-9	2-nitro- <i>m</i> -xylene N185
79-16-3	<i>N</i> -methylacetamide M150	81-49-2	1-amino-2,4-dibromanthraquinone A125
79-19-6	thiosemicarbazide T144	81-64-1	quinizarin Q7
79-20-9	methyl acetate M151	81-81-2	warfarin W1
79-21-0	peracetic acid P51	81-82-3	coumachlor C445
79-22-1	methyl chloroformate M188	81-88-9	rhodamine B R9
79-24-3	nitroethane N111	81-93-6	phenosafranin P82
79-27-6	1,1,2,2-tetrabromoethane T40	82-28-0	1-amino-2-methylanthraquinone A130
79-31-2	isobutyric acid I98	82-44-0	1-chloroanthraquinone C159
79-34-5	1,1,2,2-tetrachloroethane T50	82-66-6	diphacinone D535
79-36-7	dichloroacetyl chloride D176	82-68-8	quintozene Q12
79-38-9	chlorotrifluoroethylene C301	82-92-8	cyclizine C497
79-39-0	methacrylamide M105	83-05-6	bis(4-chlorophenyl)acetic acid B125
79-41-4	methacrylic acid M106	83-07-8	4-aminoantipyrene A113
79-42-5	thiolactic acid T132	83-26-1	pindone P193

83-32-9	acenaphthene A3	87-51-4	indole-3-acetic acid I32
83-33-0	1-indanone I20	87-52-5	gramine G44
83-34-1	3-methylindole M238	87-59-2	2,3-dimethylaniline D395
83-38-5	2,6-dichlorobenzaldehyde D187	87-60-5	3-chloro- <i>o</i> -toluidine C292
83-41-0	3-nitro- <i>o</i> -xylene N186	87-61-6	1,2,3-trichlorobenzene T241
83-42-1	6-chloro-2-nitrotoluene C233	87-62-7	2,6-dimethylaniline D398
83-66-9	musk ambrette (synthetic) M357	87-63-8	6-chloro- <i>o</i> -toluidine C297
83-67-0	theobromine T109	87-64-9	6-chloro- <i>o</i> -cresol C187
83-79-4	rotenone R18	87-65-0	2,6-dichlorophenol D238
83-86-3	phytic acid P180	87-66-1	pyrogallol P363
83-88-5	riboflavin R12	87-68-3	hexachlorobutadiene H34
83-89-6	mepacrine M55	87-69-4	L-tartaric acid T9
83-98-7	orphenadrine O35	87-86-5	pentachlorophenol P30
84-15-1	<i>o</i> -terphenyl T30	87-89-8	inositol I37
84-51-5	2-ethylanthraquinone E96	87-90-1	trichloroisocyanuric acid T250
84-60-6	anthraflavic acid A219	87-99-0	xylitol X13
84-61-7	dicyclohexyl phthalate D268	88-04-0	4-chloro-3,5-xenol C306
84-62-8	diphenyl phthalate D549	88-05-1	2,4,6-trimethylaniline T305
84-65-1	anthraquinone A220	88-06-2	2,4,6-trichlorophenol T259
84-66-2	diethyl phthalate D314	88-10-8	diethylcarbamoyl chloride D296
84-68-4	2,2'-dichlorobenzidine D191	88-12-0	<i>N</i> -vinyl-2-pyrrolidinone V37
84-69-5	diisobutyl phthalate D354	88-16-4	2-chlorobenzotrifluoride C168
84-74-2	dibutyl phthalate D160	88-21-1	aniline-2-sulfonic acid A211
84-75-3	dihexyl phthalate D341	88-72-2	2-nitrotoluene N179
84-76-4	dinonyl phthalate D508	88-73-3	2-chloronitrobenzene C222
84-77-5	didecyl phthalate D275	88-74-4	2-nitroaniline N74
84-80-0	phytomenadione P181	88-75-5	2-nitrophenol N130
84-86-6	4-aminonaphthalene-1-sulfonic acid A132	88-85-7	dinoseb D510
85-00-7	diquat dibromide D561	88-89-1	picric acid P187
85-01-8	phenanthrene P59	88-96-0	phthalamide P171
85-34-7	chlorfenac C124	88-99-3	phthalic acid P172
85-41-6	phthalamide P175	89-25-8	1-phenyl-3-methyl-5-pyrazolone P121
85-43-8	tetrahydrophthalic anhydride T76	89-32-7	pyromellitic dianhydride P364
85-44-9	phthalic anhydride P173	89-59-8	4-chloro-2-nitrotoluene C232
85-68-7	benzyl butyl phthalate B94	89-61-2	2,5-dichloronitrobenzene D229
85-73-4	phthalylsulfathiazole P177	89-62-3	4-methyl-2-nitroaniline M261
85-86-9	C.I. Solvent Red 23 C422	89-63-4	4-chloro-2-nitroaniline C221
85-98-3	<i>N,N'</i> -diethylcarbanilide D297	89-64-5	4-chloro-2-nitrophenol C229
86-00-0	2-nitrobiphenyl N98	89-72-5	2- <i>sec</i> -butylphenol B275
86-30-6	<i>N</i> -nitrosodiphenylamine N155	89-79-2	isopulegol I134
86-50-0	azinphos-methyl A264	89-83-8	thymol T154
86-55-5	1-naphthoic acid N15	89-87-2	4-nitro- <i>m</i> -xylene N187
86-57-7	1-nitronaphthalene N128	89-98-5	2-chlorobenzaldehyde C161
86-73-7	fluorene F49	90-00-6	2-ethylphenol E160
86-74-8	carbazole C64	90-02-8	salicylaldehyde S4
86-86-2	1-naphthylacetamide N21	90-04-0	2-anisidine A213
86-87-3	1-naphthylacetic acid N22	90-12-0	1-methylnaphthalene M257
86-88-4	1-naphthylthiourea N27	90-13-1	1-chloronaphthalene C217
87-10-5	3,4',5-tribromosalicylanilide T208	90-15-3	1-naphthol N17
87-28-5	glycol salicylate G38	90-39-1	sparteine S105
87-29-6	cinnamyl anthranilate C347	90-41-5	2-aminobiphenyl A119
87-40-1	2,4,6-trichloroanisole T239	90-43-7	2-phenylphenol P125

90-47-1	xanthone X3	93-15-2	methyleugenol M223
90-65-3	penicillic acid P21	93-58-3	methyl benzoate M161
90-72-2	2,4,6-tris(dimethylaminomethyl)phenol T354	93-65-2	mecoprop M40
90-84-6	diethylpropion D315	93-71-0	allidochlor A69
90-94-8	4,4'-bis(dimethylamino)benzophenone B128	93-72-1	fenoprop F14
91-08-7	toluene 2,6-diisocyanate T177	93-75-4	thioquinox T142
91-16-7	veratrole V18	93-76-5	2,4,5-T T1
91-17-8	<i>trans</i> -decahydronaphthalene D39	93-79-8	butyl 2,4,5-trichlorophenoxyacetate B279
91-17-8	<i>cis</i> -decahydronaphthalene D38	93-89-0	ethyl benzoate E99
91-20-3	naphthalene N9	93-99-2	phenyl benzoate P94
91-22-5	quinoline Q9	94-09-7	benzocaine B55
91-23-6	2-nitroanisole N77	94-11-1	2,4-D, isopropyl ester D11
91-53-2	ethoxyquin E85	94-13-3	propylparaben P336
91-56-5	isatin I78	94-17-7	4-chlorobenzoyl peroxide C171
91-57-6	2-methylnaphthalene M258	94-20-2	chlorpropamide C311
91-58-7	2-chloronaphthalene C218	94-26-8	butylparaben B269
91-59-8	2-naphthylamine N24	94-36-0	benzoyl peroxide B83
91-62-3	6-methylquinoline M301	94-52-0	5(6)-nitrobenzimidazole N86
91-63-4	quinaldine Q4	94-58-6	dihydrosafrole D347
91-64-5	coumarin C447	94-59-7	safrole S2
91-66-7	<i>N,N</i> -diethylaniline D291	94-62-2	piperine P203
91-76-9	benzoguanamine B62	94-70-2	<i>o</i> -phenetidine P71
91-80-5	methapyrilene M117	94-74-6	MCPA M32
91-93-0	3,3'-dimethoxybenzidine 4,4'-diisocyanate D379	94-75-7	2,4-D D1
91-94-1	3,3'-dichlorobenzidine D192	94-78-0	phenazopyridine P62
92-04-6	2-chloro-4-phenylphenol C249	94-79-1	2,4-D, <i>sec</i> -butyl ester D5
92-06-8	<i>m</i> -terphenyl T29	94-80-4	2,4-D, butyl ester D4
92-13-7	pilocarpine P189	94-81-5	MCPB M34
92-24-0	naphthacene N6	94-82-6	2,4-DB D25
92-36-4	2-(4-aminophenyl)-6-methylbenzothiazole A145	94-96-2	2-ethyl-1,3-hexanediol E126
92-43-3	phenidone P76	95-06-7	sulfallate S135
92-52-4	biphenyl B113	95-13-6	indene I23
92-59-1	<i>N</i> -ethyl- <i>N</i> -benzylaniline E100	95-14-7	benzotriazole B78
92-67-1	4-aminobiphenyl A121	95-15-8	benzo[<i>b</i>]thiophene B77
92-69-3	4-phenylphenol P127	95-16-9	benzothiazole B76
92-71-7	2,5-diphenyloxazole D548	95-19-2	2-heptadecyl-2-imidazoline-1-ethanol H17
92-77-3	Naphthol AS N19	95-47-6	<i>o</i> -xylene X6
92-82-0	phenazine P61	95-48-7	<i>o</i> -cresol C458
92-83-1	xanthene X1	95-49-8	2-chlorotoluene C288
92-84-2	phenothiazine P83	95-50-1	1,2-dichlorobenzene D188
92-86-4	4,4'-dibromobiphenyl D125	95-51-2	2-chloroaniline C154
92-87-5	benzidine B52	95-52-3	2-fluorotoluene F76
92-93-3	4-nitrobiphenyl N100	95-53-4	<i>o</i> -toluidine T185
92-94-4	<i>p</i> -terphenyl T31	95-54-5	<i>o</i> -phenylenediamine P102
93-00-5	6-aminonaphthalene-2-sulfonic acid A134	95-55-6	2-aminophenol A142
93-05-0	<i>N,N</i> -diethyl- <i>p</i> -phenylenediamine D313	95-57-8	2-chlorophenol C239
93-09-4	2-naphthoic acid N16	95-59-0	2,3-dichloro- <i>p</i> -dioxane D207
93-14-1	guaiphenesin G47	95-63-6	1,2,4-trimethylbenzene T307
		95-64-7	3,4-dimethylaniline D399
		95-68-1	2,4-dimethylaniline D396
		95-69-2	4-chloro- <i>o</i> -toluidine C294
		95-70-5	2,5-diaminotoluene D88

95-73-8	2,4-dichlorotoluene	D253	97-64-3	ethyl lactate	E141
95-74-9	3-chloro- <i>p</i> -toluidine	C293	97-65-4	itaconic acid	I144
95-75-0	3,4-dichlorotoluene	D255	97-74-5	monothiourea	M348
95-76-1	3,4-dichloroaniline	D182	97-77-8	disulfiram	D565
95-78-3	2,5-dimethylaniline	D397	97-85-8	isobutyl isobutyrate	I91
95-79-4	5-chloro- <i>o</i> -toluidine	C296	97-86-9	isobutyl methacrylate	I92
95-80-7	2,4-diaminotoluene	D87	97-88-1	butyl methacrylate	B267
95-82-9	2,5-dichloroaniline	D180	97-90-5	ethylene glycol dimethacrylate	E119
95-83-0	4-chloro- <i>o</i> -phenylenediamine	C245	97-95-0	2-ethyl-1-butanol	E103
95-85-2	2-amino-4-chlorophenol	A124	97-96-1	2-ethylbutyraldehyde	E104
95-86-3	2,4-diaminophenol	D81	97-99-4	tetrahydrofurfuryl alcohol	T74
95-87-4	2,5-xyleneol	X11	98-00-0	furfuryl alcohol	F127
95-92-1	diethyl oxalate	D312	98-01-1	2-furaldehyde	F120
95-93-2	durene	D602	98-04-4	phenyltrimethylammonium iodide	P139
95-94-3	1,2,4,5-tetrachlorobenzene	T46	98-05-5	phenylarsonic acid	P93
95-95-4	2,4,5-trichlorophenol	T258	98-06-6	<i>tert</i> -butylbenzene	B247
96-09-3	styrene oxide	S127	98-07-7	benzotrichloride	B79
96-12-8	1,2-dibromo-3-chloropropane	D128	98-08-8	benzotrifluoride	B80
96-13-9	2,3-dibromopropanol	D137	98-09-9	benzenesulfonyl chloride	B48
96-14-0	3-methylpentane	M274	98-13-5	phenyltrichlorosilane	P137
96-17-3	2-methylbutyraldehyde	M183	98-15-7	3-chlorobenzotrifluoride	C169
96-18-4	1,2,3-trichloropropane	T264	98-16-8	3-aminobenzotrifluoride	A118
96-19-5	1,2,3-trichloro-1-propene	T265	98-46-4	3-nitrobenzotrifluoride	N94
96-22-0	diethyl ketone	D307	98-47-5	3-nitrobenzenesulfonic acid	N84
96-23-1	1,3-dichloro-2-propanol	D247	98-51-1	4- <i>tert</i> -butyltoluene	B278
96-24-2	3-chloro-1,2-propanediol	C265	98-54-4	4- <i>tert</i> -butylphenol	B276
96-29-7	methyl ethyl ketone oxime	M221	98-56-6	4-chlorobenzotrifluoride	C170
96-32-2	methyl bromoacetate	M171	98-59-9	<i>p</i> -toluenesulfonyl chloride	T180
96-33-3	methyl acrylate	M153	98-73-7	4- <i>tert</i> -butylbenzoic acid	B249
96-34-4	methyl chloroacetate	M186	98-82-8	cumene	C474
96-37-7	methylcyclopentane	M204	98-83-9	α -methylstyrene	M307
96-41-3	cyclopentanol	C524	98-85-1	<i>sec</i> -phenethyl alcohol	P68
96-45-7	ethylenethiourea	E122	98-86-2	acetophenone	A21
96-47-9	2-methyltetrahydrofuran	M308	98-87-3	benzylidene chloride	B98
96-48-0	γ -butyrolactone	B288	98-88-4	benzoyl chloride	B82
96-66-2	4,4'-thiobis(5- <i>tert</i> -butyl- <i>o</i> -cresol)	T119	98-92-0	nicotinamide	N53
96-69-5	4,4'-thiobis(5- <i>tert</i> -butyl- <i>m</i> -cresol)	T118	98-94-2	<i>N,N</i> -dimethylcyclohexylamine	D411
96-76-4	2,4-di- <i>tert</i> -butylphenol	D155	98-95-3	nitrobenzene	N82
96-91-3	2-amino-4,6-dinitrophenol	A126	98-96-4	pyrazinamide	P348
96-96-8	4-methoxy-2-nitroaniline	M143	99-04-7	<i>m</i> -toluic acid	T181
97-00-7	1-chloro-2,4-dinitrobenzene	C194	99-05-8	3-aminobenzoic acid	A116
97-02-9	2,4-dinitroaniline	D467	99-08-1	3-nitrotoluene	N180
97-17-6	dichlofenthion	D167	99-09-2	3-nitroaniline	N75
97-18-7	2,2'-thiobis(4,6-dichlorophenol)	T122	99-26-3	bismuth subgallate	B131
97-23-4	dichlorophenol	D235	99-30-9	dicloran	D260
97-24-5	2,2'-thiobis(4-chlorophenol)	T121	99-35-4	1,3,5-trinitrobenzene	T329
97-52-9	2-methoxy-4-nitroaniline	M141	99-51-4	4-nitro- <i>o</i> -xylene	N188
97-53-0	eugenol	E187	99-52-5	2-methyl-4-nitroaniline	M259
97-54-1	isoeugenol	I102	99-54-7	3,4-dichloronitrobenzene	D230
97-56-3	C.I. Solvent Yellow 3	C424	99-55-8	2-methyl-5-nitroaniline	M260
97-62-1	ethyl isobutyrate	E139	99-56-9	4-nitro- <i>o</i> -phenylenediamine	N134
97-63-2	ethyl methacrylate	E145	99-57-0	2-amino-4-nitrophenol	A138

99-59-2	2-methoxy-5-nitroaniline M142	100-75-4	nitrosopiperidine N172
99-61-6	3-nitrobenzaldehyde N81	100-79-8	solketal S101
99-65-0	1,3-dinitrobenzene D471	100-88-9	cyclamic acid C495
99-66-1	valproic acid V8	100-97-0	hexamethylenetetramine H57
99-76-3	methylparaben M272	101-02-0	triphenyl phosphite T339
99-80-9	<i>N</i> -methyl- <i>N</i> ,4-dinitrosoaniline M207	101-05-3	anilazine A208
99-86-5	α -terpinene T34	101-14-4	4,4'-methylenebis(2-chloroaniline) M210
99-87-6	<i>p</i> -cymene C540	101-20-2	triclocarban T270
99-89-8	4-isopropylphenol I130	101-21-3	chlorpropham C312
99-91-2	4'-chloroacetophenone C149	101-25-7	<i>N,N'</i> -dinitrosopentamethylenetetramine D495
99-94-5	<i>p</i> -toluic acid T183	101-27-9	barban B4
99-98-9	<i>N,N</i> -dimethyl- <i>p</i> -phenylenediamine D448	101-31-5	hyoscyamine H124
99-99-0	4-nitrotoluene N181	101-41-7	methyl phenylacetate M286
100-00-5	4-chloronitrobenzene C224	101-42-8	fenuron F27
100-01-6	4-nitroaniline N76	101-54-2	<i>N</i> -phenyl- <i>p</i> -phenylenediamine P128
100-02-7	4-nitrophenol N132	101-55-3	4-bromodiphenyl ether B174
100-07-2	4-anisoyl chloride A217	101-61-1	4,4'-methylenebis(<i>N,N</i> -dimethylaniline) M212
100-10-7	4-(dimethylamino)benzaldehyde D387	101-67-7	4,4'-dioctyldiphenylamine D516
100-14-1	4-nitrobenzyl chloride N97	101-68-8	4,4'-methylenebis(phenyl isocyanate) M214
100-15-2	<i>N</i> -methyl-4-nitroaniline M263	101-77-9	4,4'-methylenedianiline M218
100-16-3	4-nitrophenylhydrazine N136	101-80-4	4,4'-oxydianiline O58
100-17-4	4-nitroanisole N79	101-81-5	diphenylmethane D547
100-19-6	4'-nitroacetophenone N73	101-83-7	dicyclohexylamine D265
100-21-0	terephthalic acid T26	101-84-8	diphenyl ether D544
100-22-1	<i>N,N,N',N'</i> -tetramethyl- <i>p</i> -phenylenediamine T92	101-90-6	resorcinol diglycidyl ether R6
100-25-4	1,4-dinitrobenzene D472	101-96-2	<i>N,N'</i> -di- <i>sec</i> -butyl- <i>p</i> -phenylenediamine D158
100-36-7	<i>N,N</i> -diethylethylenediamine D305	102-02-3	1-phenylbiguanide P95
100-37-8	2-diethylaminoethanol D289	102-06-7	1,3-diphenylguanidine D545
100-39-0	benzyl bromide B92	102-08-9	thiocarbanilide T123
100-40-3	4-vinyl-1-cyclohexene V31	102-36-3	3,4-dichlorophenyl isocyanate D241
100-41-4	ethylbenzene E97	102-50-1	<i>m</i> -cresidine C454
100-42-5	styrene S126	102-54-5	ferrocene F32
100-43-6	4-vinylpyridine V36	102-69-2	tripropylamine T342
100-44-7	benzyl chloride B95	102-70-5	triallylamine T199
100-46-9	benzylamine B90	102-71-6	triethanolamine T276
100-47-0	benzonitrile B68	102-76-1	triacetin T196
100-48-1	4-cyanopyridine C489	102-81-8	2-dibutylaminoethanol D143
100-50-5	1,2,3,6-tetrahydrobenzaldehyde T71	102-82-9	tributylamine T210
100-51-6	benzyl alcohol B89	102-98-7	phenylmercuric borate P117
100-52-7	benzaldehyde B40	103-03-7	phenicarbazine P75
100-54-9	3-cyanopyridine C488	103-11-7	2-ethylhexyl acrylate E131
100-56-1	phenylmercuric chloride P118	103-23-1	di- <i>sec</i> -octyl adipate D514
100-57-2	phenylmercuric hydroxide P119	103-33-3	azobenzene A268
100-61-8	<i>N</i> -methylaniline M156	103-45-7	phenethyl acetate P66
100-63-0	phenylhydrazine P108	103-50-4	dibenzyl ether D120
100-66-3	anisole A216	103-56-0	cinnamyl propionate C349
100-69-6	2-vinylpyridine V35	103-65-1	propylbenzene P324
100-70-9	2-cyanopyridine C487	103-69-5	<i>N</i> -ethylaniline E95
100-71-0	2-ethylpyridine E166		
100-73-2	acrolein dimer A36		
100-74-3	4-ethylmorpholine E152		

103-71-9	phenyl isocyanate P113	106-40-1	4-bromoaniline B160
103-72-0	phenyl isothiocyanate P115	106-42-3	<i>p</i> -xylene X7
103-73-1	phenetole P73	106-43-4	4-chlorotoluene C290
103-80-0	phenylacetyl chloride P91	106-44-5	<i>p</i> -cresol C459
103-83-3	<i>N,N</i> -dimethylbenzylamine D403	106-46-7	1,4-dichlorobenzene D190
103-84-4	acetanilide A11	106-47-8	4-chloroaniline C156
103-85-5	phenylthiourea P136	106-48-9	4-chlorophenol C241
103-90-2	paracetamol P6	106-49-0	<i>p</i> -toluidine T187
104-12-1	4-chlorophenyl isocyanate C248	106-50-3	<i>p</i> -phenylenediamine P103
104-15-4	<i>p</i> -toluenesulfonic acid T179	106-51-4	<i>p</i> -benzoquinone B74
104-40-5	4-nonylphenol N197	106-63-8	isobutyl acrylate I88
104-51-8	butylbenzene B246	106-68-3	ethyl amyl ketone E91
104-55-2	cinnamaldehyde C346	106-87-6	(±)-4-vinyl-1-cyclohexene diepoxide V32
104-65-4	cinnamyl formate C348	106-88-7	1,2-epoxybutane E36
104-72-3	decylbenzene D44	106-89-8	epichlorohydrin E33
104-74-5	laurylpyridinium chloride L10	106-90-1	glycidyl acrylate G29
104-75-6	2-ethylhexylamine E132	106-91-2	glycidyl methacrylate G31
104-76-7	2-ethylhexanol E128	106-92-3	allyl glycidyl ether A84
104-78-9	3-diethylaminopropylamine D290	106-93-4	1,2-dibromoethane D132
104-80-3	2,5-tetrahydrofuran dimethanol T73	106-94-5	1-bromopropane B185
104-83-6	4-chlorobenzyl chloride C174	106-95-6	allyl bromide A76
104-85-8	<i>p</i> -tolunitrile T190	106-97-8	butane B199
104-90-5	5-ethyl-2-picoline E163	106-98-9	1-butene B215
104-91-6	4-nitrosophenol N170	106-99-0	1,3-butadiene B197
104-93-8	4-methylanisole M157	107-00-6	1-butyne B281
104-94-9	4-anisidine A215	107-02-8	acrolein A35
105-05-5	1,4-diethylbenzene D294	107-03-9	1-propanethiol P294
105-11-3	<i>p</i> -benzoquinone dioxime B75	107-04-0	1-bromo-2-chloroethane B170
105-30-6	2-methyl-1-pentanol M277	107-05-1	allyl chloride A78
105-33-9	4-chloro-3-hydroxybutanenitrile C203	107-06-2	1,2-dichloroethane D211
105-36-2	ethyl bromoacetate E102	107-07-3	2-chloroethanol C197
105-37-3	ethyl propionate E165	107-10-8	propylamine P323
105-39-5	ethyl chloroacetate E106	107-11-9	allylamine A74
105-45-3	methyl acetoacetate M152	107-12-0	propionitrile P312
105-46-4	<i>sec</i> -butyl acetate B234	107-13-1	acrylonitrile A43
105-54-4	ethyl butyrate E105	107-14-2	chloroacetonitrile C147
105-55-5	1,3-diethylthiourea D318	107-15-3	ethylenediamine E114
105-56-6	ethyl cyanoacetate E110	107-16-4	glycolonitrile G37
105-57-7	acetal A6	107-18-6	allyl alcohol A73
105-58-8	diethyl carbonate D298	107-19-7	propargyl alcohol P301
105-59-9	methyldiethanolamine M206	107-20-0	chloroacetaldehyde C143
105-60-2	caprolactam C55	107-21-1	ethylene glycol E116
105-64-6	diisopropyl peroxydicarbonate D360	107-22-2	glyoxal G39
105-67-9	2,4-xlenol X10	107-25-5	methyl vinyl ether M317
105-74-8	lauroyl peroxide L9	107-27-7	ethylmercury(II) chloride E143
105-99-7	dibutyl adipate D140	107-29-9	acetaldoxime A9
106-19-4	dipropyl adipate D553	107-30-2	chloromethyl methyl ether C214
106-20-7	di- <i>sec</i> -octylamine D515	107-31-3	methyl formate M226
106-24-1	geraniol G12	107-37-9	allyltrichlorosilane A94
106-31-0	butyric anhydride B286	107-39-1	2,4,4-trimethyl-1-pentene T318
106-35-4	3-heptanone H24	107-41-5	2-methyl-2,4-pentanediol M275
106-37-6	1,4-dibromobenzene D124	107-44-8	sarin S8

107-46-0	hexamethyldisiloxane	H53	108-78-1	melamine	M47
107-49-3	tetraethyl pyrophosphate	T68	108-80-5	cyanuric acid	C491
107-66-4	dibutyl hydrogen phosphate	D147	108-82-7	2,6-dimethyl-4-heptanol	D418
107-70-0	4-methoxy-4-methyl-2-pentanone	M140	108-83-8	diisobutyl ketone	D353
107-71-1	<i>tert</i> -butyl peracetate	B270	108-84-9	<i>sec</i> -hexyl acetate	H77
107-72-2	amyltrichlorosilane	A206	108-86-1	bromobenzene	B161
107-82-4	1-bromo-3-methylbutane	B179	108-87-2	methylcyclohexane	M197
107-83-5	2-methylpentane	M273	108-88-3	toluene	T173
107-87-9	methyl propyl ketone	M292	108-89-4	4-picoline	P185
107-88-0	1,3-butanediol	B203	108-90-7	chlorobenzene	C163
107-89-1	aldol	A63	108-91-8	cyclohexylamine	C514
107-92-6	butyric acid	B285	108-93-0	cyclohexanol	C508
107-98-2	1-methoxy-2-propanol	M147	108-94-1	cyclohexanone	C509
108-01-0	2-dimethylaminoethanol	D388	108-95-2	phenol	P80
108-03-2	1-nitropropane	N138	108-98-5	benzenethiol	B50
108-05-4	vinyl acetate	V26	108-99-6	3-picoline	P184
108-07-6	methylmercury(II) acetate	M250	109-02-4	<i>N</i> -methylmorpholine	M255
108-09-8	1,3-dimethylbutylamine	D404	109-06-8	2-picoline	P183
108-10-1	methyl isobutyl ketone	M241	109-08-0	2-methylpyrazine	M293
108-11-2	4-methyl-2-pentanol	M281	109-09-1	2-chloropyridine	C279
108-16-7	1-dimethylamino-2-propanol	D390	109-13-7	<i>tert</i> -butyl peroxyisobutyrate	B272
108-18-9	diisopropylamine	D358	109-19-3	butyl isovalerate	B265
108-20-3	diisopropyl ether	D359	109-21-7	butyl butyrate	B250
108-21-4	isopropyl acetate	I120	109-52-4	valeric acid	V2
108-22-5	isopropenyl acetate	I118	109-53-5	isobutyl vinyl ether	I96
108-23-6	isopropyl chloroformate	I124	109-55-7	3-dimethylaminopropylamine	D392
108-24-7	acetic anhydride	A13	109-57-9	allylthiourea	A93
108-29-2	γ -valerolactone	V3	109-59-1	2-isopropoxyethanol	I119
108-30-5	succinic anhydride	S129	109-60-4	propyl acetate	P322
108-31-6	maleic anhydride	M13	109-61-5	propyl chloroformate	P326
108-34-9	diethyl 3-methylpyrazol-5-yl phosphate	D311	109-63-7	boron trifluoride diethyl etherate	B148
108-38-3	<i>m</i> -xylene	X5	109-65-9	1-bromobutane	B164
108-39-4	<i>m</i> -cresol	C457	109-66-0	pentane	P39
108-41-8	3-chlorotoluene	C289	109-67-1	1-pentene	P43
108-42-9	3-chloroaniline	C155	109-69-3	butyl chloride	B251
108-43-0	3-chlorophenol	C240	109-70-6	1-bromo-3-chloropropane	B172
108-44-1	<i>m</i> -toluidine	T184	109-73-9	butylamine	B239
108-45-2	<i>m</i> -phenylenediamine	P101	109-74-0	butyronitrile	B289
108-46-3	resorcinol	R5	109-76-2	1,3-diaminopropane	D84
108-47-4	2,4-lutidine	L62	109-77-3	malononitrile	M18
108-48-5	2,6-lutidine	L64	109-79-5	1-butanethiol	B211
108-50-9	2,6-dimethylpyrazine	D454	109-83-1	2-(methylamino)ethanol	M155
108-60-1	DCIP	D26	109-84-2	2-hydrazinoethanol	H91
108-62-3	metaldehyde	M94	109-86-4	2-methoxyethanol	M134
108-65-6	1-methoxy-2-propanol acetate	M148	109-87-5	dimethoxymethane	D382
108-67-8	mesitylene	M90	109-89-7	diethylamine	D288
108-68-9	3,5-xylene	X12	109-90-0	ethyl isocyanate	E140
108-69-0	3,5-dimethylaniline	D400	109-92-2	ethyl vinyl ether	E181
108-70-3	1,3,5-trichlorobenzene	T243	109-93-3	divinyl ether	D581
108-71-4	3,5-diaminotoluene	D93	109-94-4	ethyl formate	E123
108-77-0	cyanuric chloride	C492	109-95-5	ethyl nitrite	E156
			109-97-7	pyrrole	P366

109-99-9	tetrahydrofuran T72	111-27-3	1-hexanol H65
110-00-9	furan F123	111-30-8	glutaraldehyde G21
110-01-0	tetrahydrothiophene T77	111-31-9	1-hexanethiol H63
110-02-1	thiophene T139	111-34-2	butyl vinyl ether B280
110-05-4	di- <i>tert</i> -butyl peroxide D150	111-36-4	butyl isocyanate B264
110-12-3	5-methyl-2-hexanone M233	111-40-0	diethylenetriamine D303
110-13-4	2,5-hexanedione H62	111-42-2	diethanolamine D281
110-15-6	succinic acid S128	111-43-3	dipropyl ether D557
110-16-7	maleic acid M12	111-44-4	bis(2-chloroethyl) ether B120
110-17-8	fumaric acid F115	111-46-6	diethylene glycol D301
110-18-9	<i>N,N,N',N'</i> -tetramethylethylenediamine T89	111-48-8	2,2'-thiodiethanol T129
110-19-0	isobutyl acetate I87	111-49-9	hexamethyleneimine H56
110-22-5	diacetyl peroxide D66	111-65-9	octane O9
110-32-7	bis(2-hexyloxyethyl) adipate B129	111-69-3	adiponitrile A49
110-43-0	2-heptanone H23	111-71-7	heptanal H19
110-44-1	sorbic acid S102	111-76-2	2-butoxyethanol B226
110-46-3	isoamyl nitrite I81	111-77-3	2-(2-methoxyethoxy)ethanol M135
110-49-6	2-methoxyethyl acetate M136	111-78-4	1,5-cyclooctadiene C519
110-54-3	hexane H60	111-84-2	nonane N193
110-57-6	<i>trans</i> -1,4-dichloro-2-butene D201	111-87-5	1-octanol O13
110-58-7	pentylamine P47	111-88-6	1-octanethiol O10
110-60-1	1,4-butanediamine B201	111-91-1	bis(2-chloroethoxy)methane B118
110-61-2	succinonitrile S130	111-92-2	dibutylamine D141
110-62-3	valeraldehyde V1	111-94-4	3,3'-iminodipropionitrile I13
110-63-4	1,4-butanediol B204	111-96-6	diglyme D338
110-65-6	1,4-butyndiol B282	112-04-9	octadecyltrichlorosilane O4
110-66-7	amyl mercaptan A201	112-07-2	2-butoxyethyl acetate B229
110-68-9	<i>N</i> -methylbutylamine M180	112-12-9	2-undecanone U6
110-69-0	butyraldoxime B284	112-15-2	2-(2-ethoxyethoxy)ethanol acetate E77
110-71-4	1,2-dimethoxyethane D381	112-24-3	triethylenetetramine T284
110-74-7	propyl formate P331	112-27-6	triethylene glycol T280
110-75-8	2-chloroethyl vinyl ether C199	112-30-1	1-decanol D42
110-78-1	propyl isocyanate P333	112-31-2	decanal D40
110-80-5	2-ethoxyethanol E76	112-34-5	2-(2-butoxyethoxy)ethanol B227
110-82-7	cyclohexane C507	112-35-6	triethylene glycol monomethyl ether T283
110-83-8	cyclohexene C511	112-36-7	2-ethoxyethyl ether E80
110-85-0	piperazine P200	112-37-8	undecanoic acid U4
110-86-1	pyridine P357	112-40-3	dodecane D585
110-87-2	dihydropyran D346	112-42-5	1-undecanol U5
110-88-3	1,3,5-trioxane T333	112-44-7	undecanal U1
110-89-4	piperidine P201	112-48-1	1,2-dibutoxyethane D138
110-91-8	morpholine M353	112-49-2	triglyme T296
110-93-0	6-methyl-5-hepten-2-one M232	112-53-8	1-dodecanol D588
110-96-3	diisobutylamine D352	112-54-9	dodecanal D584
110-97-4	diisopropanolamine D356	112-55-0	1-dodecanethiol D586
111-02-4	squalene S109	112-57-2	tetraethylenepentamine T65
111-13-7	2-octanone O16	112-60-7	tetraethylene glycol T64
111-14-8	heptanoic acid H22	112-62-9	<i>Z</i> -methyl oleate M270
111-15-9	2-ethoxyethyl acetate E79	112-79-8	(<i>E</i>)-oleic acid O30
111-20-6	sebacic acid S11	112-80-1	(<i>Z</i>)-oleic acid O31
111-24-0	1,5-dibromopentane D136	112-84-5	erucamide E46
		112-90-3	oleamine O28

112-92-5	stearyl alcohol	S113	118-96-7	2,4,6-trinitrotoluene	T331
113-52-0	imipramine hydrochloride	I15	119-04-0	neomycin B	N36
113-92-8	chlorpheniramine maleate	C308	119-06-2	ditridecyl phthalate	D577
114-07-8	erythromycin	E47	119-07-3	octyl decyl phthalate	O22
114-26-1	propoxur	P315	119-12-0	pyridaphenthion	P355
114-33-0	N-methyl-3-pyridinecarboxamide	M297	119-26-6	2,4-dinitrophenylhydrazine	D491
114-49-8	hyoscine bromide	H123	119-28-8	8-aminonaphthalene-2-sulfonic acid	A136
114-86-3	phenformin	P74	119-32-4	4-methyl-3-nitroaniline	M262
115-02-6	azaserine	A260	119-33-5	2-nitro- <i>p</i> -cresol	N104
115-07-1	propene	P303	119-34-6	4-amino-2-nitrophenol	A140
115-10-6	dimethyl ether	D413	119-36-8	methyl salicylate	M305
115-11-7	isobutene	I86	119-38-0	isolan	I107
115-18-4	2-methyl-3-buten-2-ol	M178	119-61-9	benzophenone	B70
115-19-5	2-methyl-3-butyne-2-ol	M182	119-64-2	tetralin	T80
115-21-9	ethyltrichlorosilane	E180	119-65-3	isoquinoline	I135
115-26-4	dimefox	D367	119-79-9	5-aminonaphthalene-2-sulfonic acid	A133
115-27-5	chlorendic anhydride	C123	119-90-4	<i>o</i> -dianisidine	D95
115-28-6	chlorendic acid	C122	119-93-7	<i>o</i> -tolidine	T172
115-29-7	endosulfan	E19	120-11-6	benzyl isoeugenol	B99
115-32-2	dicofol	D261	120-12-7	anthracene	A218
115-77-5	pentaerythritol	P35	120-23-0	(2-naphthylthio)acetic acid	N26
115-78-6	chlorphonium chloride	C309	120-32-1	2-benzyl-4-chlorophenol	B96
115-86-6	triphenyl phosphate	T337	120-36-5	dichlorprop	D257
115-90-2	fensulfothion	F23	120-40-1	lauramide DEA	L7
115-96-8	tris(2-chloroethyl) phosphate	T350	120-47-8	ethylparaben	E158
116-01-8	ethoate-methyl	E71	120-51-4	benzyl benzoate	B91
116-06-3	aldicarb	A62	120-58-1	isosafrole	I136
116-14-3	tetrafluoroethylene	T70	120-61-6	dimethyl terephthalate	D459
116-15-4	hexafluoropropene	H48	120-62-7	sulfoxide	S148
116-16-5	hexachloroacetone	H32	120-71-8	<i>p</i> -cresidine	C455
116-29-0	tetradifon	T63	120-72-9	indole	I31
116-54-1	methyl dichloroacetate	M205	120-73-0	purine	P346
117-10-2	danthron	D22	120-75-2	2-methylbenzothiazole	M162
117-18-0	tecnazene	T14	120-78-5	2,2'-dithiobis(benzothiazole)	D572
117-39-5	quercetin	Q2	120-80-9	catechol	C95
117-52-2	fumarin	F116	120-82-1	1,2,4-trichlorobenzene	T242
117-79-3	2-aminoanthraquinone	A112	120-83-2	2,4-dichlorophenol	D237
117-80-6	dichlone	D169	120-92-3	cyclopentanone	C525
117-81-7	dioctyl phthalate	D519	121-14-2	2,4-dinitrotoluene	D499
117-82-8	bis(2-methoxyethyl) phthalate	B130	121-17-5	4-chloro-3-nitrobenzotrifluoride	C225
117-83-9	bis(2-butoxyethyl) phthalate	B116	121-20-0	cinerin II	C345
117-84-0	di- <i>n</i> -octyl phthalate	D520	121-21-1	pyrethrin I	P352
118-52-5	1,3-dichloro-5,5-dimethylhydantoin	D205	121-29-9	pyrethrin II	P353
118-55-8	phenyl salicylate	P132	121-33-5	vanillin	V17
118-61-6	ethyl salicylate	E169	121-43-7	trimethyl borate	T308
118-69-4	2,6-dichlorotoluene	D254	121-44-8	triethylamine	T278
118-74-1	hexachlorobenzene	H33	121-45-9	trimethyl phosphite	T325
118-75-2	chloranil	C115	121-46-0	2,5-norbornadiene	N202
118-79-6	2,4,6-tribromophenol	T207	121-47-1	metanilic acid	M97
118-90-1	<i>o</i> -toluic acid	T182	121-54-0	benzethonium chloride	B51
118-91-2	2-chlorobenzoic acid	C165	121-57-3	sulfanilic acid	S138
118-92-3	2-aminobenzoic acid	A115	121-66-4	2-amino-5-nitrothiazole	A141

121-69-7	<i>N,N</i> -dimethylaniline	D394	123-86-4	butyl acetate	B233
121-73-3	3-chloronitrobenzene	C223	123-91-1	1,4-dioxane	D530
121-75-5	malathion	M11	123-92-2	isoamyl acetate	I80
121-79-9	propyl gallate	P332	123-93-3	thiodiglycolic acid	T130
121-82-4	RDX	R2	123-96-6	2-octanol	O14
121-87-9	2-chloro-4-nitroaniline	C220	124-02-7	diallylamine	D70
121-88-0	2-amino-5-nitrophenol	A139	124-04-9	adipic acid	A48
121-91-5	isophthalic acid	I113	124-07-2	octanoic acid	O12
121-92-6	3-nitrobenzoic acid	N88	124-09-4	hexamethylenediamine	H54
122-03-2	4-isopropylbenzaldehyde	I122	124-13-0	octanal	O8
122-09-8	phentermine	P88	124-17-4	2-(2-butoxyethoxy)ethanol acetate	B228
122-14-5	fenitrothion	F11	124-18-5	decane	D41
122-15-6	dimetan	D370	124-19-6	nonanal	N192
122-18-9	cetyldimethylbenzylammonium chloride	C103	124-20-9	spermidine	S106
122-20-3	triisopropanolamine	T297	124-25-4	myristyl aldehyde	M363
122-34-9	simazine	S37	124-30-1	stearamine	S111
122-39-4	diphenylamine	D540	124-38-9	carbon dioxide	C74
122-42-9	propham	P305	124-40-3	dimethylamine	D384
122-51-0	triethyl orthoformate	T286	124-48-1	dibromochloromethane	D126
122-52-1	triethyl phosphite	T288	124-64-1	tetrakis(hydroxymethyl)phosphonium chloride	T79
122-60-1	glycidyl phenyl ether	G35	124-65-2	sodium dimethylarsinate	S63
122-66-7	1,2-diphenylhydrazine	D546	124-87-8	picrotoxin	P188
122-88-3	4-CPA	C452	125-12-2	isobornyl acetate	I83
122-99-6	2-phenoxyethanol	P86	125-28-0	dihydrocodeine	D344
123-01-3	1-phenyldodecane	P100	125-33-7	primidone	P272
123-03-5	cetylpyridinium chloride	C104	125-69-9	dextromethorphan hydrobromide	D64
123-05-7	2-ethylhexanal	E125	125-71-3	dextromethorphan	D63
123-07-9	4-ethylphenol	E162	126-06-7	3-bromo-1-chloro-5,5-dimethylhydantoin	B169
123-15-9	2-methylvaleraldehyde	M316	126-07-8	griseofulvin	G46
123-19-3	4-heptanone	H25	126-11-4	tris(hydroxymethyl)nitromethane	T357
123-20-6	vinyl butyrate	V29	126-22-7	butonate	B224
123-23-9	disuccinoyl peroxide	D564	126-30-7	neopentyl glycol	N40
123-28-4	dilauryl 3,3'-thiodipropionate	D365	126-33-0	sulfolane	S143
123-30-8	4-aminophenol	A144	126-72-7	tris(2,3-dibromopropyl) phosphate	T352
123-31-9	hydroquinone	H107	126-73-8	tributyl phosphate	T212
123-32-0	2,5-dimethylpyrazine	D452	126-75-0	demeton-S	D53
123-33-1	maleic hydrazide	M14	126-85-2	mechlorethamine <i>N</i> -oxide	M39
123-35-3	myrcene	M361	126-98-7	methacrylonitrile	M108
123-38-6	propionaldehyde	P309	126-99-8	chloroprene	C262
123-39-7	<i>N</i> -methylformamide	M225	127-00-4	1-chloro-2-propanol	C266
123-42-2	diacetone alcohol	D65	127-09-3	sodium acetate	S40
123-51-3	3-methyl-1-butanol	M174	127-17-3	pyruvic acid	P368
123-54-6	acetylacetone	A22	127-18-4	tetrachloroethylene	T51
123-62-6	propionic anhydride	P311	127-19-5	<i>N,N</i> -dimethylacetamide	D383
123-63-7	paraldehyde	P9	127-20-8	dalapon-sodium	D20
123-72-8	butyraldehyde	B283	127-31-1	fluorocortisone	F63
123-73-9	crotonaldehyde	C467	127-33-3	demeclocycline	D47
123-75-1	pyrrolidine	P367	127-41-3	α -ionone	I57
123-76-2	levulinic acid	L40	127-63-9	phenyl sulfone	P134
123-77-3	azodicarbonamide	A271	127-65-1	chloramine T	C113
123-79-5	di- <i>n</i> -octyl adipate	D513			

127-69-5	sulfisoxazole S141	133-53-9	2,4-dichloro-3,5-xyleneol D256
127-82-2	zinc <i>p</i> -phenolsulfonate Z13	133-90-4	chloramben C110
127-85-5	sodium arsanilate S43	134-03-2	sodium ascorbate S46
127-90-2	bis(2,3,3,3-tetrachloropropyl) ether B136	134-31-6	hydroxyquinoline sulfate H120
127-91-3	β -pinene P198	134-32-7	1-naphthylamine N23
128-03-0	potassium dimethyldithiocarbamate P247	134-62-3	<i>N,N</i> -diethyl- <i>m</i> -toluamide D319
128-04-1	sodium dimethyldithiocarbamate S64	134-72-5	ephedrine sulfate E31
128-37-0	butylated hydroxytoluene B245	134-80-5	diethylpropion hydrochloride D316
128-39-2	2,6-di- <i>tert</i> -butylphenol D156	135-01-3	1,2-diethylbenzene D292
128-56-3	sodium anthraquinone-1-sulfonate S42	135-19-3	2-naphthol N18
128-66-5	C.I. Vat Yellow 4 C428	135-20-6	cupferron C476
128-95-0	1,4-diaminoanthraquinone D76	135-23-9	methapyrilene hydrochloride M118
129-00-0	pyrene P351	135-88-6	<i>N</i> -phenyl-2-naphthylamine P124
129-06-6	warfarin sodium W3	136-25-4	2-(2,4,5-trichlorophenoxy)ethyl 2,2-dichloropropionate T261
129-15-7	2-methyl-1-nitroanthraquinone M264		phenazopyridine hydrochloride P63
129-17-9	C.I. Acid Blue 1 C386	136-40-3	dipropyl 2,5-pyridinedicarboxylate D559
129-20-4	oxyphenbutazone O63	136-45-8	2,4-DES-sodium D57
129-44-2	1,5-diaminoanthraquinone D77	136-78-7	5-methylbenzotriazole M165
129-67-9	endothal sodium E23	136-85-6	methyl 2-cyanoacrylate M196
129-79-3	2,4,7-trinitrofluorenone T330	137-05-3	2,4-diaminophenol dihydrochloride D82
129-99-7	sodium mercurhydrin S77	137-09-7	2,4,5-trimethylaniline T304
130-15-4	1,4-naphthoquinone N20	137-17-7	thiram T147
130-17-6	2-(4-aminophenyl)-6-methyl-7-benzothiazolesulfonic acid A146	137-26-8	ziram Z19
130-80-3	stilbestrol dipropionate S117	137-30-4	metam-sodium M96
130-95-0	quinine Q6	137-42-8	lignocaine L43
131-01-1	deserpidine D58	137-58-6	2,4-dinonylphenol D507
131-09-9	2-chloroanthraquinone C160	137-99-5	butyl lactate B266
131-11-3	dimethyl phthalate D450	138-22-7	phenyltrimethylammonium chloride P138
131-14-6	2,6-diaminoanthraquinone D78	138-24-9	4-nitrobenzenesulfonic acid N85
131-16-8	dipropyl phthalate D558	138-42-1	shikimic acid S26
131-17-9	diallyl phthalate D72	138-59-0	limonene L45
131-18-0	dipentyl phthalate D534	138-86-3	<i>N,N</i> -dimethyl-4-nitrosoaniline D445
131-52-2	sodium pentachlorophenolate S82	138-89-6	sodium phenolate S85
131-54-4	2,2'-dihydroxy-4,4'-dimethoxybenzophenone D349	139-02-6	sodium cyclamate S59
131-55-5	2,2',4,4'-tetrahydroxybenzophenone T78	139-05-9	nitrilotriacetic acid N70
131-56-6	4-benzoylresorcinol B85	139-13-9	EDTA disodium salt E7
131-70-4	monobutyl phthalate M341	139-33-3	propazine P302
131-73-7	dipicrylamine D550	139-40-2	4,4'-thiodianiline T127
131-74-8	ammonium picrate A182	139-65-1	furaltadone F122
131-89-5	2-cyclohexyl-4,6-dinitrophenol C516	139-91-3	nithiazide N63
131-91-9	1-nitroso-2-naphthol N167	139-94-6	benzyl acetate B88
132-27-4	sodium <i>o</i> -phenylphenolate S86	140-11-4	1,5-diphenylcarbazine D542
132-32-1	3-amino-9-ethylcarbazole A128	140-22-7	benzathine B45
132-53-6	2-nitroso-1-naphthol N168	140-28-3	benzyl cyanide B97
132-64-9	dibenzofuran D111	140-29-4	<i>N</i> -aminoethylpiperazine A129
132-66-1	naptalam N30	140-31-8	acinitrazole A31
133-06-2	captan C59	140-40-9	monuron-TCA M351
133-07-3	folpet F97	140-41-0	4-(chloroacetyl)acetanilide C150
133-32-4	indole-3-butyric acid I34	140-49-8	fenaminosulf F2
133-37-9	DL-tartaric acid T8	140-56-7	aramite A232
		140-57-8	4-allylanisole A75
		140-67-0	

140-76-1	2-methyl-5-vinylpyridine	M319	148-79-8	thiabendazole	T111
140-79-4	dinitrosopiperazine	D496	148-82-3	melfhalan	M49
140-88-5	ethyl acrylate	E89	149-29-1	patulin	P16
140-93-2	proxan-sodium	P343	149-30-4	2-mercaptobenzothiazole	M61
141-01-5	iron(II) fumarate	I72	149-57-5	2-ethylhexanoic acid	E127
141-04-8	diisobutyl adipate	D351	149-73-5	trimethyl orthoformate	T313
141-17-3	dibutoxyethoxyethyl adipate	D139	149-74-6	dichloromethylphenylsilane	D224
141-28-6	diethyl adipate	D287	150-05-0	D-adrenaline	A50
141-32-2	butyl acrylate	B238	150-13-0	4-aminobenzoic acid	A117
141-43-5	ethanolamine	E62	150-38-9	EDTA trisodium salt	E9
141-59-3	<i>tert</i> -octanethiol	O11	150-46-9	ethyl borate	E101
141-66-2	dicrotophos	D263	150-50-5	merphos	M89
141-75-3	butyryl chloride	B290	150-68-5	monuron	M350
141-78-6	ethyl acetate	E87	150-69-6	4-ethoxyphenylurea	E81
141-79-7	mesityl oxide	M91	150-76-5	4-methoxyphenol	M144
141-82-2	malonic acid	M17	151-21-3	sodium lauryl sulfate	S76
141-90-2	2-thiouracil	T145	151-38-2	2-methoxyethylmercury acetate	M137
141-93-5	1,3-diethylbenzene	D293	151-50-8	potassium cyanide	P245
141-94-6	hexetidine	H75	151-56-4	aziridine	A266
141-97-9	ethyl acetoacetate	E88	151-67-7	halothane	H4
142-04-1	aniline hydrochloride	A210	152-16-9	schradan	S9
142-28-9	1,3-dichloropropane	D246	153-18-4	rutin	R22
142-29-0	cyclopentene	C527	153-94-6	D-tryptophan	T368
142-46-1	2,5-dithiobiurea	D573	154-41-6	norephedrine hydrochloride	N203
142-59-6	nabam	N1	154-69-8	tripelennamine hydrochloride	T334
142-62-1	hexanoic acid	H64	154-93-8	1,3-bis(chloroethyl)-1-nitrosourea	B121
142-71-2	copper acetate	C430	155-04-4	zinc 2-mercaptobenzothiazole	Z10
142-73-4	iminodiacetic acid	I11	156-08-1	benzphetamine	B86
142-82-5	heptane	H20	156-10-5	4-nitrosodiphenylamine	N154
142-84-7	dipropylamine	D554	156-43-4	<i>p</i> -phenetidine	P72
142-96-1	dibutyl ether	D145	156-51-4	phenelzine sulfate	P64
143-07-7	lauric acid	L8	156-59-2	<i>cis</i> -1,2-dichloroethylene	D213
143-08-8	1-nonanol	N195	156-60-5	<i>trans</i> -1,2-dichloroethylene	D214
143-33-9	sodium cyanide	S58	156-62-7	calcium cyanamide	C29
143-50-0	chlordecone	C119	189-55-9	dibenzo[<i>a,i</i>]pyrene	D117
143-67-9	vinblastine sulfate	V21	189-64-0	dibenzo[<i>a,h</i>]pyrene	D116
144-19-4	2,2,4-trimethyl-1,3-pentanediol	T315	191-24-2	benzo[<i>ghi</i>]perylene	B69
144-21-8	DSMA	D601	191-26-4	dibenzo[<i>cd,jk</i>]pyrene	D119
144-41-2	morphothion	M354	191-30-0	dibenzo[<i>a,l</i>]pyrene	D118
144-49-0	fluoroacetic acid	F55	192-65-4	dibenzo[<i>a,e</i>]pyrene	D115
144-62-7	oxalic acid	O46	192-97-2	benzo[<i>e</i>]pyrene	B72
145-13-1	pregnenolone	P270	193-39-5	indeno[1,2,3- <i>cd</i>]pyrene	I24
145-73-3	endothal	E22	194-59-2	7 <i>H</i> -dibenzo[<i>c,g</i>]carbazole	D104
146-22-5	nitrazepam	N67	198-55-0	perylene	P57
146-48-5	(+)-yohimbine	Y1	203-12-3	benzo[<i>ghi</i>]fluoranthene	B57
147-14-8	phthalocyanine blue	P176	203-64-5	4 <i>H</i> -cyclopenta[<i>def</i>]phenanthrene	C526
147-24-0	diphenhydramine hydrochloride	D538	205-43-6	benzo[<i>b</i>]naphtho[1,2- <i>d</i>]thiophene	B65
147-85-3	L-proline	P284	205-82-3	benzo[<i>j</i>]fluoranthene	B58
147-94-4	cytarabine	C546	205-99-2	benzo[<i>b</i>]fluoranthene	B56
148-01-6	dinitolmide	D465	206-44-0	fluoranthene	F48
148-18-5	dithiocarb	D575	207-08-9	benzo[<i>k</i>]fluoranthene	B59
148-24-3	8-hydroxyquinoline	H119	208-96-8	acenaphthylene	A4

217-59-4	triphenylene T336	305-01-1	esculetin E48
218-01-9	chrysene C340	305-03-3	chlorambucil C111
224-42-0	dibenz[<i>a,j</i>]acridine D102	305-33-9	iproniazid phosphate I63
226-36-8	dibenz[<i>a,h</i>]acridine D101	306-37-6	1,2-dimethylhydrazine dihydrochloride D422
239-35-0	benzo[<i>b</i>]naphtho[2,1- <i>d</i>]thiophene B66	309-00-2	aldrin A65
243-46-9	benzo[<i>b</i>]naphtho[2,3- <i>d</i>]thiophene B67	311-45-5	paraoxon P10
244-63-3	β-carboline C71	311-89-7	perfluorotributylamine P55
244-69-9	γ-carboline C72	314-13-6	Evans Blue E190
244-76-8	α-carboline C70	314-40-9	bromacil B151
260-94-6	acridine A34	315-14-0	2,4,6-trifluoronitrobenzene T293
262-12-4	dibenzo- <i>p</i> -dioxin D106	315-18-4	mexacarbate M331
271-44-3	indazole I22	315-22-0	monocrotaline M342
271-89-6	benzofuran B61	315-30-0	allopurinol A70
281-23-2	adamantane A47	316-42-7	emetine hydrochloride E17
285-67-6	6-oxabicyclo[3.1.0]hexane O43	317-34-0	aminophylline A147
287-92-3	cyclopentane C522	319-78-8	D-isoleucine I108
288-13-1	pyrazole P349	320-67-2	5-azacytidine A257
288-32-4	imidazole I9	324-93-6	4'-fluoro-4-aminobiphenyl F57
288-47-1	thiazole T114	327-98-0	trichloronate T253
288-88-0	1,2,4-triazole T204	328-39-2	DL-leucine L36
291-64-5	cycloheptane C505	329-71-5	2,5-dinitrophenol D487
297-76-7	ethynodiol diacetate E182	330-54-1	diuron D579
297-78-9	isobenzan I82	330-55-2	linuron L50
297-97-2	thionazin T135	331-39-5	caffeic acid C19
298-00-0	parathion-methyl P14	333-41-5	diazinon D99
298-02-2	phorate P145	334-88-3	diazomethane D100
298-03-3	demeton-O D51	336-59-4	heptafluorobutyric anhydride H18
298-04-4	disulfoton D566	348-54-9	2-fluoroaniline F58
298-07-7	di- <i>sec</i> -octyl phosphate D518	348-67-4	D-methionine M124
298-18-0	DL-1,2,3,4-diepoxybutane D279	351-83-7	4'-fluoroacetanilide F54
298-46-4	carbamazepine C61	352-32-9	4-fluorotoluene F77
298-81-7	methoxsalen M129	352-93-2	ethyl sulfide E172
299-42-3	ephedrine E30	353-36-6	fluoroethane F64
299-45-6	<i>O,O</i> -diethyl <i>O</i> -(4-methylcoumarin-7-yl)phosphorothioate D309	353-42-4	boron trifluoride dimethyl etherate B149
299-75-2	treosulfan T195	353-50-4	carbonyl fluoride C80
299-78-5	allylisopropylacetamide A86	353-59-3	bromochlorodifluoromethane B168
299-84-3	fenchlorfos F8	357-57-3	brucine B191
299-86-5	crufomate C471	359-06-8	fluoroacetyl chloride F56
300-62-9	amphetamine A193	359-83-1	pentazocine P42
300-76-5	naled N3	360-89-4	octafluoro-2-butene O5
301-04-2	lead acetate L12	366-70-1	ibenzmethylin hydrochloride I1
301-12-2	oxydemeton-methyl O57	367-12-4	2-fluorophenol F68
302-01-2	hydrazine H87	367-25-9	2,4-difluoroaniline D329
302-15-8	methylhydrazine sulfate M235	370-50-3	flucufuron F42
302-17-0	chloral hydrate C108	371-40-4	4-fluoroaniline F60
302-22-7	chlormadinone acetate C139	371-41-5	4-fluorophenol F70
302-27-2	aconitine A33	371-62-0	2-fluoroethanol F65
302-84-1	DL-serine S24	372-19-0	3-fluoroaniline F59
303-34-4	lasiocarpine L6	372-20-3	3-fluorophenol F69
303-47-9	ochratoxin A O1	379-52-2	triphenyltin fluoride T341
304-20-1	hydralazine hydrochloride H85	379-79-3	ergotamine tartrate E44

382-21-8	octafluoroisobutene	O6	481-42-5	plumbagin	P216
384-22-5	2-nitrobenzotrifluoride	N93	481-72-1	aloe emodin	A95
389-08-2	nalidixic acid	N4	482-89-3	Indigo	I25
390-64-7	prenylamine	P271	483-63-6	crotamiton	C466
396-01-0	triarterene	T203	484-31-1	dill apiole	D366
398-32-3	<i>N</i> -(4'-fluorobiphen-4-yl)acetamide	F62	485-31-4	binapacryl	B111
402-54-0	4-nitrobenzotrifluoride	N95	485-47-2	ninhydrin	N60
407-25-0	trifluoroacetic anhydride	T291	486-25-9	9-fluorenone	F50
409-02-9	methylheptenone	M231	486-66-8	daidzein	D18
409-21-2	silicon carbide	S31	486-84-0	harmene	H6
420-04-2	cyanamide	C479	488-10-8	jasmone	J3
420-12-2	ethylene sulfide	E121	488-23-3	1,2,3,4-tetramethylbenzene	T87
421-20-5	methyl fluorosulfonate	M224	491-11-2	3-chloro-4-nitrophenol	C228
431-03-8	2,3-butanedione	B209	491-35-0	4-methylquinoline	M299
434-07-1	oxymetholone	O62	492-17-1	2,4'-diphenyldiamine	D543
434-13-9	lithocholic acid	L56	492-62-6	α -glucose	G16
439-14-5	diazepam	D98	493-01-6	<i>cis</i> -decahydronaphthalene	D38
442-51-3	harmine	H7	493-02-7	<i>trans</i> -decahydronaphthalene	D39
443-48-1	metronidazole	M327	493-52-7	Methyl Red	M304
446-72-0	genistein	G9	494-03-1	chlornaphazine	C142
446-86-6	azathioprine	A261	494-19-9	iminodibenzyl	I12
453-17-8	D-glyceraldehyde	G24	494-38-2	C.I. Solvent Orange 15	C421
456-59-7	cyclandelate	C496	494-44-0	7-aminonaphthalene-2-sulfonic acid	A135
458-24-2	fenfluramine	F9	495-48-7	azoxybenzene	A274
458-37-7	curcumin	C478	495-54-5	2,4-diaminoazobenzene	D79
460-19-5	cyanogen	C482	495-69-2	hippuric acid	H81
462-06-6	fluorobenzene	F61	495-73-8	benquinox	B35
462-08-8	3-aminopyridine	A152	496-11-7	indan	I17
462-95-3	diethoxymethane	D286	496-72-0	3,4-diaminotoluene	D92
463-51-4	ketene	K8	497-18-7	carbohydrazide	C69
463-58-1	carbonyl sulfide	C81	497-19-8	sodium carbonate	S52
463-71-8	thiophosgene	T140	497-23-4	2(5 <i>H</i>)-furanone	F124
463-82-1	neopentane	N39	498-60-2	3-furaldehyde	F121
464-10-8	tribromonitromethane	T206	500-28-7	chlorthion	C320
464-48-2	(-)-camphor	C52	501-65-5	diphenylacetylene	D539
464-49-3	(+)-camphor	C51	502-39-6	methylmercury(II) dicyandiamide	M251
465-42-9	capsanthin	C56	502-55-6	dixan	D582
465-73-6	isodrin	I101	502-65-8	lycopene	L65
469-21-6	doxylamine	D598	503-09-3	epifluorohydrin	E34
469-62-5	propoxyphene	P318	503-17-3	crotonylene	C469
470-38-2	capsorubin	C57	503-30-0	trimethylene oxide	T309
470-82-6	cineole	C343	503-74-2	isovaleric acid	I141
470-90-6	chlorfenvinphos	C128	504-20-1	phorone	P147
471-34-1	calcium carbonate	C25	504-24-5	4-aminopyridine	A153
472-93-5	γ -carotene	C90	504-29-0	2-aminopyridine	A151
474-86-2	equilin	E41	504-60-9	1,3-pentadiene	P34
475-81-0	D-glaucine	G15	504-61-0	<i>trans</i> -2-buten-1-ol	B218
479-13-0	coumestrol	C449	504-88-1	3-nitropropionic acid	N140
479-45-8	nitramine	N65	505-22-6	1,3-dioxane	D529
479-61-8	chlorophyll a	C253	505-60-2	mustard gas	M359
480-30-8	dichloralphenazone	D170	506-30-9	eicosanoic acid	E13
480-41-1	naringenin	N31	506-32-1	arachidonic acid	A231

506-61-6	potassium silver cyanide	P262	528-74-5	dichloromethotrexate	D223
506-64-9	silver cyanide	S35	529-19-1	<i>o</i> -tolunitrile	T189
506-68-3	cyanogen bromide	C483	529-34-0	α -tetralone	T83
506-77-4	cyanogen chloride	C484	530-93-8	β -tetralone	T84
506-78-5	cyanogen iodide	C485	531-59-9	7-methoxycoumarin	M133
506-87-6	ammonium carbonate	A168	531-76-0	merphalan	M88
506-93-4	guanidine nitrate	G49	531-82-8	<i>N</i> -[4-(5-nitro-2-furyl)-2-thiazolyl]acetamide	N117
506-96-7	acetyl bromide	A24	532-03-6	methocarbamol	M125
507-02-8	acetyl iodide	A27	532-27-4	2-chloroacetophenone	C148
507-09-5	thioacetic acid	T116	532-82-1	chrysoidin	C341
507-20-0	<i>tert</i> -butyl chloride	B253	533-45-9	clomethiazole	C360
507-60-8	scilliroside	S10	533-74-4	dazomet	D24
507-70-0	borneol	B143	534-07-6	1,3-dichloroacetone	D174
508-77-0	cymarin	C536	534-15-6	1,1-dimethoxyethane	D380
509-14-8	tetranitromethane	T95	534-22-5	2-methylfuran	M228
510-15-6	chlorobenzilate	C164	534-52-1	4,6-dinitro- <i>o</i> -cresol	D475
512-56-1	trimethyl phosphate	T324	535-13-7	ethyl 2-chloropropionate	E108
513-35-9	amylene	A200	535-77-3	<i>m</i> -cymene	C538
513-37-1	1-chloro-2-methylpropene	C215	535-89-7	crimidine	C463
513-38-2	1-iodo-2-methylpropane	I53	536-33-4	ethionamide	E69
513-42-8	2-methyl-2-propen-1-ol	M289	536-50-5	α ,4-dimethylbenzyl alcohol	D402
513-48-4	2-iodobutane	I47	536-75-4	4-ethylpyridine	E168
513-77-9	barium carbonate	B9	536-78-7	3-ethylpyridine	E167
513-85-9	2,3-butanediol	B205	536-90-3	3-anisidine	A214
513-88-2	1,1-dichloroacetone	D173	538-07-8	HN1	H82
514-10-3	abietic acid	A2	538-23-8	tricaprylin	T224
514-73-8	dithiazanine iodide	D571	538-75-0	dicyclohexylcarbodiimide	D267
514-78-3	C.I. Food Orange 8	C413	538-86-3	methyl benzyl ether	M166
516-06-3	DL-valine	V5	540-18-1	amyl butyrate	A197
517-28-2	hematoxylin	H14	540-37-4	4-iodoaniline	I44
518-47-8	C.I. Acid Yellow 73	C399	540-38-5	4-iodophenol	I55
518-75-2	citrinin	C353	540-42-1	isobutyl propionate	I95
518-82-1	emodin	E18	540-54-5	1-chloropropane	C263
518-83-2	1,3-dihydroxyanthraquinone	D348	540-63-6	ethanedithiol	E59
519-23-3	ellipticine	E15	540-67-0	ethyl methyl ether	E147
519-62-0	chlorophyll b	C254	540-73-8	1,2-dimethylhydrazine	D421
519-63-1	chlorophyll d	C256	540-82-9	ethylsulfuric acid	E173
520-26-3	hesperidine	H30	540-84-1	2,2,4-trimethylpentane	T314
523-80-8	apiole	A230	540-88-5	<i>tert</i> -butyl acetate	B235
524-81-2	mebhydrolin	M36	541-09-3	uranyl acetate	U10
525-66-6	propranolol	P321	541-25-3	Lewisite	L41
525-79-1	kinetin	K11	541-41-3	ethyl chloroformate	E107
525-82-6	flavone	F36	541-53-7	2,4-dithiobiuret	D574
526-08-9	sulfaphenazole	S139	541-69-5	<i>m</i> -phenylenediamine dihydrochloride	P104
526-55-6	tryptophol	T370	541-73-1	1,3-dichlorobenzene	D189
526-73-8	1,2,3-trimethylbenzene	T306	541-85-5	5-methyl-3-heptanone	M230
527-53-7	1,2,3,5-tetramethylbenzene	T88	542-55-2	isobutyl formate	I90
527-54-8	3,4,5-trimethylphenol	T323	542-59-6	ethylene glycol acetate	E117
527-60-6	2,4,6-trimethylphenol	T322	542-62-1	barium cyanide	B12
527-73-1	2-nitroimidazole	N124	542-69-8	1-iodobutane	I46
527-84-4	<i>o</i> -cymene	C539			
528-29-0	1,2-dinitrobenzene	D470			

542-75-6	1,3-dichloropropene	D250	558-25-8	methanesulfonyl fluoride	M114
542-76-7	3-chloropropionitrile	C274	562-10-7	doxylamine succinate	D599
542-78-9	malonaldehyde	M16	563-12-2	ethion	E68
542-88-1	bis(chloromethyl) ether	B123	563-41-7	semicarbazide hydrochloride	S22
542-90-5	ethyl thiocyanate	E175	563-45-1	3-methyl-1-butene	M175
542-92-7	1,3-cyclopentadiene	C528	563-47-3	3-chloro-2-methylpropene	C216
543-59-9	amyl chloride	A198	563-52-0	3-chloro-1-butene	C178
543-80-6	barium acetate	B6	563-54-2	1,2-dichloropropene	D249
543-90-8	cadmium acetate	C3	563-58-6	1,1-dichloropropene	D248
544-18-3	cobalt(II) formate	C373	563-68-8	thallium(I) acetate	T101
544-25-2	cycloheptatriene	C506	563-80-4	methyl isopropyl ketone	M244
544-63-8	myristic acid	M362	564-00-1	<i>meso</i> -1,2,3,4-diepoxybutane	D280
544-92-3	copper(I) cyanide	C435	564-94-3	myrtenal	M365
544-97-8	dimethylzinc	D461	565-48-0	<i>cis</i> -1,8-terpin	T33
545-06-2	trichloroacetonitrile	T229	565-67-3	2-methyl-3-pentanol	M278
545-55-1	tris(1-aziridinyl)phosphine oxide	T346	565-80-0	2,4-dimethyl-3-pentanone	D447
546-67-8	lead tetraacetate	L32	569-41-5	1,8-dimethylnaphthalene	D439
547-58-0	Methyl Orange	M271	569-57-3	chlorotrianisene	C299
547-63-7	methyl isobutyrate	M242	569-61-9	C.I. Basic Red 9	C402
547-64-8	methyl lactate	M247	569-64-2	Malachite Green	M9
551-74-6	mannomustine hydrochloride	M29	571-58-4	1,4-dimethylnaphthalene	D435
552-16-9	2-nitrobenzoic acid	N87	571-61-9	1,5-dimethylnaphthalene	D436
552-30-7	trimellitic anhydride	T299	572-48-5	coumithoate	C450
553-24-2	Neutral Red	N42	573-56-8	2,6-dinitrophenol	D488
553-69-5	phenyramidol	P140	573-98-8	1,2-dimethylnaphthalene	D433
554-00-7	2,4-dichloroaniline	D179	574-12-9	isoflavone	I104
554-12-1	methyl propionate	M290	575-37-1	1,7-dimethylnaphthalene	D438
554-84-7	3-nitrophenol	N131	575-41-7	1,3-dimethylnaphthalene	D434
555-03-3	3-nitroanisole	N78	575-43-9	1,6-dimethylnaphthalene	D437
555-30-6	methyldopa	M208	576-24-9	2,3-dichlorophenol	D236
555-31-7	aluminium isopropoxide	A101	577-11-7	docusate sodium	D583
555-37-3	neburon	N32	577-19-5	2-bromonitrobenzene	B180
555-77-1	tris(2-chloroethyl)amine	T349	577-71-9	3,4-dinitrophenol	D489
555-84-0	nifuradene	N58	578-54-1	2-ethylaniline	E92
556-24-1	methyl isovalerate	M246	578-94-9	diphenylamine chloroarsine	D541
556-52-5	glycidol	G28	579-44-2	benzoin	B64
556-56-9	allyl iodide	A85	580-51-8	3-phenylphenol	P126
556-61-6	methyl isothiocyanate	M245	581-40-8	2,3-dimethylnaphthalene	D440
556-64-9	methyl thiocyanate	M310	581-42-0	2,6-dimethylnaphthalene	D441
556-82-1	3-methyl-2-buten-1-ol	M176	581-88-4	debrisoquine	D36
556-88-7	nitroguanidine	N122	581-89-5	2-nitronaphthalene	N129
557-05-1	zinc stearate	Z16	582-16-1	2,7-dimethylnaphthalene	D442
557-17-5	methyl propyl ether	M291	583-15-3	mercury benzoate	M67
557-20-0	diethylzinc	D322	583-39-1	2-mercaptobenzimidazole	M60
557-21-1	zinc cyanide	Z8	583-57-3	1,2-dimethylcyclohexane	D409
557-31-3	allyl ethyl ether	A82	583-59-5	2-methylcyclohexanol	M199
557-34-6	zinc acetate	Z3	583-60-8	2-methylcyclohexanone	M203
557-40-4	diallyl ether	D71	583-61-9	2,3-lutidine	L61
557-75-5	vinyl alcohol	V27	583-63-1	<i>o</i> -benzoquinone	B73
557-98-2	2-chloropropene	C271	584-79-2	allethrin	A68
558-13-4	carbon tetrabromide	C77	584-84-9	toluene 2,4-diisocyanate	T176
558-17-8	2-iodo-2-methylpropane	I54	586-06-1	orci prenataline	O33

586-62-9	terpinolene T37	598-56-1	<i>N,N</i> -dimethylethylamine D414
586-78-7	4-bromonitrobenzene B181	598-77-6	1,1,2-trichloropropane T263
587-02-0	3-ethylaniline E93	598-78-7	2-chloropropionic acid C272
587-04-2	3-chlorobenzaldehyde C162	598-92-5	1-chloro-1-nitroethane C226
588-22-7	3,4-dichlorophenoxyacetic acid D239	599-79-1	sulfasalazine S140
588-59-0	stilbene S115	600-14-6	2,3-pentanedione P40
589-16-2	4-ethylaniline E94	600-25-9	1-chloro-1-nitropropane C231
589-38-8	3-hexanone H68	601-77-4	<i>N</i> -nitrosodiisopropylamine N152
589-63-9	4-octanone O17	602-01-7	2,3-dinitrotoluene D498
589-91-3	4-methylcyclohexanol M201	602-38-0	1,8-dinitronaphthalene D483
589-93-5	2,5-lutidine L63	602-87-9	5-nitroacenaphthene N71
589-98-0	3-octanol O15	603-34-9	triphenylamine T335
590-00-1	potassium sorbate P263	603-35-0	triphenylphosphine T338
590-01-2	butyl propionate B277	604-59-1	α -naphthoflavone N13
590-17-0	bromoacetonitrile B159	604-75-1	oxazepam O48
590-18-1	<i>cis</i> -2-butene B216	605-71-0	1,5-dinitronaphthalene D482
590-86-3	isovaleraldehyde I140	606-20-2	2,6-dinitrotoluene D501
590-88-5	1,3-butanediamine B200	606-21-3	2-chloro-1,3-dinitrobenzene C195
590-96-5	methylazoxymethanol M159	606-22-4	2,6-dinitroaniline D468
591-08-2	1-acetyl-2-thiourea A29	606-23-5	1,3-indandione I18
591-23-1	3-methylcyclohexanol M200	606-37-1	1,3-dinitronaphthalene D481
591-27-5	3-aminophenol A143	607-57-8	2-nitrofluorene N114
591-50-4	iodobenzene I45	608-27-5	2,3-dichloroaniline D178
591-60-6	butyl acetoacetate B236	608-31-1	2,6-dichloroaniline D181
591-78-6	2-hexanone H67	608-73-1	HCH H9
591-87-7	allyl acetate A72	608-93-5	pentachlorobenzene P27
591-97-9	1-chloro-2-butene C176	609-06-3	L-xylitol X15
592-01-8	calcium cyanide C30	609-20-1	2,6-dichloro- <i>p</i> -phenylenediamine D240
592-04-1	mercury(II) cyanide M72	609-89-2	2,4-dichloro-6-nitrophenol D233
592-05-2	lead cyanide L17	609-93-8	2,6-dinitro- <i>p</i> -cresol D474
592-34-7	butyl chloroformate B254	610-39-9	3,4-dinitrotoluene D502
592-41-6	1-hexene H70	611-06-3	2,4-dichloronitrobenzene D228
592-62-1	methylazoxymethanol acetate M160	611-07-4	5-chloro-2-nitrophenol C230
592-76-7	1-heptene H26	611-14-3	2-ethyltoluene E176
592-84-7	butyl formate B258	611-19-8	2-chlorobenzyl chloride C172
592-85-8	mercury(II) thiocyanate M87	611-32-5	8-methylquinoline M303
592-87-0	lead thiocyanate L33	611-72-3	DL-mandelic acid M20
593-60-2	vinyl bromide V28	612-24-8	2-nitrobenzonitrile N90
593-70-4	chlorofluoromethane C200	612-60-2	7-methylquinoline M302
593-74-8	dimethylmercury D427	612-64-6	<i>N</i> -nitroso- <i>N</i> -ethylaniline N157
594-04-7	dichloriodomethane D220	612-83-9	3,3'-dichlorobenzidine dihydrochloride D193
594-18-3	dibromodichloromethane D130	612-94-2	2-phenylnaphthalene P123
594-42-3	trichloromethanesulfonyl chloride T252	613-13-8	2-aminoanthracene A111
594-72-9	1,1-dichloro-1-nitroethane D232	613-35-4	diacetylbenzidine D67
595-33-5	megestrol acetate M44	614-00-6	<i>N</i> -nitroso- <i>N</i> -methylaniline N160
597-25-1	dimethyl morpholinophosphoramidate D432	614-45-9	<i>tert</i> -butyl peroxybenzoate B271
597-64-8	tetraethyltin T69	614-78-8	<i>o</i> -tolylthiourea T193
598-14-1	ethyldichloroarsine E112	615-05-4	2,4-diaminoanisole D73
598-32-3	3-buten-2-ol B220	615-13-4	2-indanone I21
598-50-5	methylurea M315	615-22-5	2-(methylthio)benzothiazole M309
598-55-0	methyl carbamate M184	615-50-9	2,5-diaminotoluene sulfate D89

615-53-2	<i>N</i> -nitroso- <i>N</i> -methylethane N164	626-60-8	3-chloropyridine C280
615-62-3	3-chloro- <i>p</i> -cresol C182	626-67-5	1-methylpiperidine M288
615-65-6	2-chloro- <i>p</i> -toluidine C291	626-86-8	ethyl hydrogen adipate E136
615-66-7	2-chloro- <i>p</i> -phenylenediamine C242	626-89-1	4-methyl-1-pentanol M280
615-74-7	6-chloro- <i>m</i> -cresol C186	626-93-7	2-hexanol H66
616-47-7	1-methylimidazole M236	627-05-4	1-nitrobutane N101
617-89-0	furfurylamine F128	627-11-2	2-chloroethyl chloroformate C198
617-94-7	2-phenyl-2-propanol P131	627-12-3	<i>n</i> -propyl carbamate P325
618-62-2	3,5-dichloronitrobenzene D231	627-13-4	propyl nitrate P334
618-85-9	3,5-dinitrotoluene D503	627-27-0	3-buten-1-ol B219
618-87-1	3,5-dinitroaniline D469	627-30-5	3-chloropropanol C268
619-08-9	2-chloro-4-nitrophenol C227	627-44-1	diethylmercury D308
619-15-8	2,5-dinitrotoluene D500	627-63-4	fumaryl chloride F117
619-17-0	4-nitroanthranilic acid N80	628-20-6	4-chlorobutyronitrile C180
619-24-9	3-nitrobenzonitrile N91	628-32-0	1-ethoxypropane E82
619-72-7	4-nitrobenzonitrile N92	628-63-7	amyl acetate A195
619-73-8	4-nitrobenzyl alcohol N96	628-76-2	1,5-dichloropentane D234
620-14-4	3-ethyltoluene E177	628-81-9	butyl ethyl ether B257
620-17-7	3-ethylphenol E161	628-86-4	mercury fulminate M73
620-20-2	3-chlorobenzyl chloride C173	628-96-6	ethylene dinitrate E115
620-22-4	<i>m</i> -tolunitrile T188	629-14-1	1,2-diethoxyethane D285
621-64-7	<i>N</i> -nitrosodipropylamine N156	629-20-9	cyclooctatetraene C521
622-58-2	<i>p</i> -tolyl isocyanate T192	630-08-0	carbon monoxide C76
622-96-8	4-ethyltoluene E178	630-10-4	selenourea S21
623-15-4	2-furfurylidene acetone F129	630-20-6	1,1,1,2-tetrachloroethane T49
623-26-7	terephthalonitrile T27	630-60-4	ouabain O40
623-30-3	β -furylacrolein F131	630-93-3	phenytoin sodium P142
623-70-1	(<i>E</i>)-ethyl crotonate E109	631-61-8	ammonium acetate A162
624-18-0	<i>p</i> -phenylenediamine dihydrochloride P105	632-21-3	1,1,3,3-tetrachloroacetone T43
624-48-6	dimethyl maleate D426	632-69-9	Rose Bengal sodium R16
624-54-4	pentyl propionate P49	632-99-5	Magenta I M1
624-64-6	<i>trans</i> -2-butene B217	633-03-4	C.I. Basic Green 1 C400
624-65-7	3-chloropropyne C278	633-96-5	C.I. Acid Orange 7 C391
624-72-6	1,2-difluoroethane D331	634-66-2	1,2,3,4-tetrachlorobenzene T44
624-83-9	methyl isocyanate M243	634-67-3	2,3,4-trichloroaniline T231
624-92-0	dimethyl disulfide D412	634-90-2	1,2,3,5-tetrachlorobenzene T45
625-16-1	<i>tert</i> -amyl acetate A196	634-91-3	3,4,5-trichloroaniline T234
625-27-4	2-methyl-2-pentene M283	634-93-5	2,4,6-trichloroaniline T233
625-28-5	isovaleronitrile I142	636-21-5	<i>o</i> -toluidine hydrochloride T186
625-33-2	3-penten-2-one P44	636-30-6	2,4,5-trichloroaniline T232
625-36-5	3-chloropropionyl chloride C275	637-07-0	clofibrate C358
625-45-6	methoxyacetic acid M130	638-11-9	isopropyl butyrate I123
625-54-7	2-ethoxypropane E83	638-21-1	phenylphosphine P129
625-55-8	isopropyl formate I126	638-23-3	carbocysteine C67
625-89-8	<i>N</i> -nitrosobis(2,2,2-trifluoroethyl)amine N145	639-58-7	triphenyltin chloride T340
626-01-7	3-iodoaniline I43	640-15-3	thiometon T134
626-17-5	isophthalonitrile I114	640-19-7	fluoroacetamide F53
626-23-3	di- <i>sec</i> -butylamine D142	640-68-6	D-valine V4
626-38-0	2-pentyl acetate P46	643-58-3	2-methylbiphenyl M169
626-43-7	3,5-dichloroaniline D183	644-08-6	4-methylbiphenyl M170
		644-64-4	dimetilan D462
		644-97-3	dichlorophenylphosphine D242

645-62-5	2-ethyl-2-hexenal E130	771-03-9	dehydroacetic acid D45
646-06-0	1,3-dioxolane D532	771-29-9	tetralin hydroperoxide T81
650-51-1	sodium trichloroacetate S97	771-51-7	indole-3-acetonitrile I33
652-67-5	isosorbide I137	782-74-1	2,2-dichlorohydrazobenzene D218
671-04-5	carbanolate C62	786-19-6	carbophenothion C82
671-16-9	procarbazine P274	789-02-6	<i>o,p'</i> -DDT D34
674-82-8	diketene D363	789-07-1	2-nitropyrene N142
675-14-9	cyanuric fluoride C493	794-93-4	dihydroxymethylfuratrizine D350
675-20-7	2-piperidinone P202	797-63-7	levonorgestrel L38
676-22-2	(<i>E,E,E</i>)-1,5,9-cyclododecatriene C503	800-24-8	aziridyl- <i>p</i> -benzoquinone A267
676-97-1	methylphosphonic dichloride M287	804-36-4	nitrovin N184
680-31-9	hexamethylphosphoramide H58	814-49-3	diethyl chlorophosphate D299
681-84-5	tetramethyl orthosilicate T91	814-68-6	acryloyl chloride A44
683-18-1	dibutyltin dichloride D161	814-78-8	3-methyl-3-buten-2-one M179
684-16-2	hexafluoroacetone H45	814-91-5	copper oxalate C439
684-93-5	1-nitroso-1-methylurea N163	815-57-6	3-methyl-2,4-pentanedione M276
687-47-8	(-)-ethyl lactate E142	815-82-7	copper tartrate C444
691-37-2	4-methyl-1-pentene M284	818-08-6	dibutyltin oxide D164
693-65-2	pentyl ether P48	822-06-0	hexamethylene diisocyanate H55
695-77-2	1,2,3,4-tetrachloro-1,3-cyclopentadiene T47	823-40-5	2,6-diaminotoluene D90
696-28-6	phenyldichloroarsine P98	824-11-3	trimethylolpropane phosphite T310
696-29-7	isopropylcyclohexane I125	828-00-2	dimethoxane D377
697-82-5	2,3,5-trimethylphenol T320	831-82-3	4-phenoxyphenol P87
700-38-9	6-nitro- <i>m</i> -cresol N107	834-12-8	ametryn A109
709-98-8	propanil P295	838-88-0	4,4'-methylenebis(2-methylaniline) M213
712-68-5	2-amino-5-(5-nitro-2-furyl)-1,3,4-thiadiazole A137	842-07-9	C.I. Solvent Yellow 14 C426
716-79-0	phenzidole P143	860-22-0	Indigo Carmine I26
719-22-2	2,6-di- <i>tert</i> -butyl- <i>p</i> -benzoquinone D144	865-21-4	vinblastine V20
719-96-0	<i>N</i> -(dichlorofluoromethylthio)phthalimide D217	867-27-6	demeton- <i>O</i> -methyl D52
720-69-4	2,4-diamino-6-(5-nitro-2-furanyl)- <i>s</i> -triazine D80	868-85-9	dimethyl phosphite D449
723-46-6	sulfamethoxazole S136	869-29-4	acrolein diacetate A37
731-27-1	tolylfluorid T191	870-08-6	diocetyl tin oxide D526
732-11-6	phosmet P153	872-50-4	<i>N</i> -methylpyrrolidone M298
732-26-3	2,4,6-tri- <i>tert</i> -butylphenol T211	874-35-1	5-methylindan M237
738-70-5	trimethoprim T302	886-50-0	terbutryn T25
739-71-9	trimipramine T328	892-21-7	3-nitrofluoranthene N113
741-58-2	bensulide B36	900-95-8	fentin acetate F25
756-79-6	dimethyl methylphosphonate D430	915-67-3	Amaranth A108
757-58-4	hexaethyl tetraphosphate H44	918-00-3	1,1,1-trichloroacetone T227
758-17-8	<i>N</i> -methyl- <i>N</i> -formylhydrazine M227	919-44-8	dimethyl (<i>Z</i>)-1-methyl-2-methylcarbamoylvinyl phosphate D429
759-73-9	1-nitroso-1-ethylurea N158	919-76-6	amidithion A110
759-94-4	EPTC E40	919-86-8	demeton- <i>S</i> -methyl D54
760-93-0	methacrylic anhydride M107	920-37-6	2-chloroacrylonitrile C152
763-29-1	2-methyl-1-pentene M282	920-46-7	methacryloyl chloride M109
763-32-6	3-methyl-3-buten-1-ol M177	920-66-1	1,1,1,3,3,3-hexafluoro-2-propanol H47
764-13-6	2,5-dimethyl-2,4-hexadiene D419	921-03-9	1,1,3-trichloroacetone T228
764-41-0	1,4-dichloro-2-butene D200	923-26-2	2-hydroxypropyl methacrylate H117
765-34-4	glycidaldehyde G27	924-16-3	<i>N</i> -nitrosodibutylamine N146
766-09-6	1-ethylpiperidine E164	924-42-5	<i>N</i> -(hydroxymethyl)acrylamide H113
		926-64-7	2-dimethylaminoacetonitrile D385
		927-07-1	<i>tert</i> -butyl peroxyphosphate B273

927-49-1	6-undecanone U7	1077-16-3	1-phenylhexane P107
927-73-1	4-chloro-1-butene C179	1079-21-6	phenylhydroquinone P110
928-45-0	butyl nitrate B268	1085-98-9	dichlofluanid D168
928-65-4	hexyltrichlorosilane H79	1111-78-0	ammonium carbamate A167
928-95-0	(E)-2-hexen-1-ol H72	1113-02-6	omethoate O32
928-96-1	(Z)-3-hexen-1-ol H74	1113-14-0	<i>trans</i> -1,2-bis(propylsulfonyl)ethylene B135
928-97-2	(E)-3-hexen-1-ol H73	1113-38-8	diammonium oxalate D94
929-06-6	2-(2-aminoethoxy)ethanol A127	1114-34-7	D-lyxose L68
930-37-0	glycidyl methyl ether G32	1114-71-2	pebulate P17
930-55-2	<i>N</i> -nitrosopyrrolidine N174	1115-70-4	metformin hydrochloride M100
933-75-5	2,3,6-trichlorophenol T257	1116-54-7	<i>N</i> -nitrosodiethanolamine N148
933-78-8	2,3,5-trichlorophenol T256	1119-94-4	dodecyltrimethylammonium bromide D592
935-95-5	2,3,5,6-tetrachlorophenol T56	1119-97-7	myristyltrimethylammonium bromide M364
936-49-2	2-phenyl-2-imidazoline P112	1120-21-4	undecane U2
937-14-4	3-chloroperbenzoic acid C237	1120-71-4	1,3-propane sultone P293
939-27-5	2-ethylnaphthalene E154	1122-60-7	nitrocyclohexane N110
944-22-9	fonofos F99	1124-33-0	4-nitropyridine 1-oxide N144
945-51-7	phenyl sulfoxide P135	1125-27-5	dichloroethylphenylsilane D215
947-02-4	phosfolan P151	1126-78-9	<i>N</i> -butylaniline B242
950-10-7	mephosfolan M56	1127-76-0	1-ethylnaphthalene E153
950-37-8	methidathion M121	1129-41-5	metolcarb M324
952-23-8	proflavine hydrochloride P280	1131-64-2	debrisoquine D36
957-51-7	diphenamid D536	1134-23-2	cycloate C498
968-81-0	acetoexamide A15	1138-52-9	3,5-di- <i>tert</i> -butylphenol D157
973-21-7	dinobuton D504	1156-19-0	tolazamide T170
989-38-8	C.I. Basic Red 1 C401	1162-65-8	aflatoxin B ₁ A53
991-42-4	norbormide N201	1163-19-5	pentabromophenyl ether P24
992-21-2	lymecycline L66	1165-39-5	aflatoxin G ₁ A55
998-30-1	triethoxysilane T277	1172-63-0	jasmolin II J2
999-61-1	2-hydroxypropyl acrylate H116	1189-85-1	<i>tert</i> -butyl chromate B255
999-81-5	chlormequat chloride C141	1191-80-6	mercury oleate M80
999-97-3	hexamethyldisilazane H52	1194-65-6	dichlobenil D166
1002-16-0	amyl nitrate A202	1208-52-2	2,4'-methylenedianiline M217
1011-73-0	2,4-dinitrophenolate sodium D490	1212-29-9	<i>N,N'</i> -dicyclohexylthiourea D269
1014-69-3	desmetryn D60	1222-05-5	galaxolide G2
1014-70-6	simetryn S38	1239-45-8	ethidium bromide E65
1022-22-6	<i>p,p'</i> -DDMU D33	1260-17-9	carminic acid C86
1024-57-3	heptachlor epoxide H16	1271-19-8	titanocene dichloride T168
1025-15-6	triallyl isocyanurate T201	1299-86-1	aluminium carbide A98
1031-07-8	endosulfan sulfate E21	1300-71-6	xlenol X9
1031-47-6	triamphos T202	1300-94-3	amyl- <i>m</i> -cresol A199
1066-30-4	chromium(III) acetate C332	1302-78-9	bentonite B39
1066-33-7	ammonium bicarbonate A165	1303-00-0	gallium arsenide G4
1066-45-1	trimethyltin chloride T327	1303-33-9	arsenic trisulfide A245
1067-29-4	tripropyltin oxide T344	1303-86-2	boron oxide B144
1069-66-5	sodium valproate S100	1303-96-4	borax B141
1070-70-8	1,4-butanediol diacrylate B207	1304-28-5	barium oxide B14
1070-78-6	1,1,1,3-tetrachloropropane T57	1304-29-6	barium peroxide B17
1071-83-6	glyphosate G40	1304-82-1	bismuth telluride B132
1072-35-1	lead distearate L20	1305-62-0	calcium hydroxide C33
1073-67-2	4-chlorostyrene C284		
1073-93-4	<i>N</i> -isopropylmaleimide I127		

1305-78-8	calcium oxide	C37	1335-31-5	mercury oxycyanide	M83
1305-79-9	calcium peroxide	C39	1335-32-6	lead subacetate	L29
1305-99-3	calcium phosphide	C41	1335-66-6	isocyclocitral	I100
1306-19-0	cadmium oxide	C11	1335-87-1	hexachloronaphthalene	H39
1306-23-6	cadmium sulfide	C14	1336-21-6	ammonium hydroxide	A176
1307-96-6	cobalt(II) oxide	C376	1338-02-9	copper naphthenate	C437
1309-37-1	iron(III) oxide	I74	1338-23-4	methyl ethyl ketone peroxide	M222
1309-48-4	magnesium oxide	M6	1338-24-5	naphthenic acid	N12
1309-60-0	lead dioxide	L19	1338-39-2	sorbitan monolaurate	S103
1309-64-4	antimony trioxide	A227	1341-49-7	ammonium hydrogen difluoride	A175
1310-58-3	potassium hydroxide	P254	1343-78-8	cochineal	C382
1310-73-2	sodium hydroxide	S73	1344-28-1	aluminium oxide	A103
1310-82-3	rubidium hydroxide	R20	1344-81-6	calcium polysulfides	C42
1313-13-9	manganese dioxide	M24	1344-95-2	calcium silicate	C43
1313-27-5	molybdenum trioxide	M339	1397-94-0	antimycin A	A228
1313-82-2	sodium sulfide	S93	1400-61-9	nystatin	N210
1314-13-2	zinc oxide	Z12	1401-55-4	tannic acid	T6
1314-20-1	thorium dioxide	T150	1404-04-2	neomycin	N34
1314-24-5	phosphorus trioxide	P167	1405-87-4	bacitracin	B1
1314-32-5	thallium(III) oxide	T107	1406-05-9	penicillin	P22
1314-34-7	vanadium trioxide	V15	1406-65-1	chlorophyll	C252
1314-56-3	phosphorus pentoxide	P163	1415-73-2	barbaloin	B3
1314-62-1	vanadium pentoxide	V12	1420-04-8	clonitralid	C362
1314-80-3	phosphorus pentasulfide	P162	1420-07-1	dinoterb	D512
1314-84-7	zinc phosphide	Z14	1421-49-4	3,5-di- <i>tert</i> -butyl-4-hydroxybenzoic acid	D148
1314-85-8	phosphorus sesquisulfide	P164		EDTPA	E11
1314-87-0	lead sulfide	L31	1429-50-1	1,2-epoxyhexane	E38
1317-35-7	manganese tetroxide	M27	1436-34-6	1-nonanethiol	N194
1317-39-1	copper(I) oxide	C440	1455-21-6	<i>N</i> -nitroso-2,6-dimethylmorpholine	N153
1317-42-6	cobalt(II) sulfide	C380	1456-28-6	tetrabutyltin	T42
1318-93-0	montmorillonite	M349	1461-25-2	1,2:3,4-diepoxybutane	D278
1319-77-3	cresol	C456	1464-53-5	<i>N</i> -(1-naphthyl)ethylenediamine	
1320-18-9	2,4-D, propylene glycol butyl ether ester	D15	1465-25-4	dihydrochloride	N25
				dimexano	D463
1320-67-8	methoxypropanol	M146	1468-37-7	5-indanol	I19
1321-64-8	pentachloronaphthalene	P29	1470-94-6	benzarone	B44
1321-74-0	divinylbenzene	D580	1477-19-6	<i>m</i> -xylylenediamine	X17
1321-94-4	methylnaphthalene	M256	1477-55-0	menthol	M53
1327-53-3	arsenic trioxide	A244	1490-04-6	benzathine penicillin	B46
1330-20-7	xylene (mixed isomers)	X8	1538-09-6	(<i>Z,Z</i>)-1,5-cyclooctadiene	C520
1330-43-4	sodium tetraborate	S96	1552-12-1	trichloro(chloromethyl)silane	T246
1330-78-5	tritoyl phosphate	T361	1558-25-4	carbofuran	C68
1331-17-5	propylene glycol allyl ether	P328	1563-66-2	decarbofuran	D43
1331-22-2	methylcyclohexanone	M202	1563-67-3	1-ethoxy-2-propanol	E84
1331-54-0	(2-ethylhexyl)phenol	E135	1569-02-4	cyclohexyl mercaptan	C518
1332-21-4	asbestos	A247	1569-69-3	4-chloro- <i>o</i> -cresol	C184
1332-40-7	copper oxychloride	C441	1570-64-5	trifluralin	T294
1332-58-7	kaolin	K2	1582-09-8	daminozide	D21
1333-74-0	hydrogen	H96	1596-84-5	mercury(II) acetate	M65
1333-82-0	chromium(VI) oxide	C337	1600-27-7	1-ethoxyethyl acetate	E78
1333-83-1	sodium hydrogen fluoride	S71	1608-72-6	prometon	P288
1333-86-4	carbon black	C73	1610-18-0		

1615-80-1	1,2-diethylhydrazine	D306	1912-26-1	trietazine	T275
1617-17-0	2-chloropropionitrile	C273	1918-00-9	dicamba	D165
1633-83-6	1,4-butane sultone	B210	1918-02-1	picloram	P182
1634-04-4	methyl <i>tert</i> -butyl ether	M181	1918-13-4	chlorthiamid	C319
1634-78-2	malaoxon	M10	1918-16-7	propachlor	P290
1639-09-4	1-heptanethiol	H21	1928-38-7	2,4-D, methyl ester	D13
1639-60-7	propoxyphene hydrochloride	P319	1928-44-5	2,4-D, octyl ester	D14
1642-54-2	diethylcarbamazine citrate	D295	1929-73-3	2,4-D, butoxyethanol ester	D3
1646-88-4	aldoxycarb	A64	1929-77-7	vernolate	V19
1649-08-7	1,2-dichloro-1,1-difluoroethane	D203	1929-82-4	nitrapyrin	N66
1658-56-6	C.I. Acid Red 88	C397	1929-88-0	benzthiazuron	B87
1675-54-3	bisphenyl A diglycidyl ether	B134	1936-15-8	C.I. Acid Orange 10	C392
1678-82-6	<i>trans</i> - <i>p</i> -menthane	M51	1937-37-7	C.I. Direct Black 38	C403
1678-91-7	ethylcyclohexane	E111	1948-33-0	<i>tert</i> -butylhydroquinone	B262
1680-21-3	triethylene glycol diacrylate	T281	1954-28-5	triethylene glycol diglycidyl ether	T282
1687-30-5	hexahydrophthalic acid	H49	1955-45-9	pivalolactone	P211
1689-82-3	C.I. Solvent Yellow 7	C425	1967-16-4	chlorbufam	C117
1689-83-4	ioxynil	I59	1982-42-9	2,4-D, amine salt	D2
1689-84-5	bromoxynil	B189	1982-49-6	siduron	S27
1693-71-6	triallyl borate	T200	1983-10-4	tributyltin fluoride	T215
1694-09-3	Benzyl Violet 4B	B101	1984-59-4	2,3-dichloroanisole	D184
1698-60-8	chloridazon	C131	1984-65-2	2,6-dichloroanisole	D185
1702-17-6	clopyralid	C364	2001-94-7	EDTA dipotassium salt	E6
1705-85-7	6-methylchrysene	M195	2001-95-8	valinomycin	V7
1712-64-7	isopropyl nitrate	I129	2008-39-1	2,4-D, dimethylamine salt	D8
1713-15-1	2,4-D, isobutyl ester	D9	2008-41-5	butylate	B243
1738-25-6	3-(dimethylamino)propionitrile	D391	2016-36-6	choline salicylate	C327
1739-84-0	1,2-dimethylimidazole	D424	2027-17-0	2-isopropyl naphthalene	I128
1746-01-6	dibenzo- <i>p</i> -dioxin, 2,3,7,8-tetrachloro-	D110	2032-59-9	aminocarb	A123
1746-81-2	monolinuron	M345	2032-65-7	methiocarb	M123
1752-30-3	acetone thiosemicarbazide	A19	2039-85-2	3-chlorostyrene	C283
1758-68-5	1,2-diaminoanthraquinone	D75	2039-87-4	2-chlorostyrene	C282
1761-71-3	dicykan	D272	2050-47-7	bis(4-bromophenyl) ether	B115
1762-95-4	ammonium thiocyanate	A190	2050-92-2	dipentylamine	D533
1768-31-6	pentachloroacetone	P25	2051-78-7	allyl butyrate	A77
1777-84-0	3-nitro- <i>p</i> -acetophenelide	N72	2052-49-5	tetrabutylammonium hydroxide	T41
1795-17-1	dodecylcyclohexane	D590	2068-78-2	vincristine sulfate	V25
1797-74-6	allyl phenylacetate	A91	2078-54-8	propofol	P314
1806-54-8	trioctyl phosphate	T332	2079-00-7	blasticidin-S	B139
1817-47-6	<i>p</i> -nitrocumene	N109	2095-06-9	<i>N,N</i> -diglycidylaniline	D336
1825-21-4	2,3,4,5,6-pentachloroanisole	P26	2097-19-0	phenylsilatrane	P133
1836-75-5	nitrofen	N112	2104-64-5	EPN	E35
1838-59-1	allyl formate	A83	2104-96-3	bromophos	B183
1861-32-1	chlorthal-dimethyl	C317	2113-58-8	3-nitrobiphenyl	N99
1861-40-1	benfluralin	B29	2122-70-5	ethyl 1-naphthylacetate	E155
1863-63-4	ammonium benzoate	A164	2136-89-2	2-chlorobenzotrithloride	C166
1866-31-5	allyl cinnamate	A80	2155-70-6	tributyltin methacrylate	T218
1879-09-0	2,4-dimethyl-6- <i>tert</i> -butylphenol	D405	2156-71-0	1-chloropiperidine	C260
1885-14-9	phenyl chloroformate	P97	2163-69-1	cycluron	C532
1888-71-7	hexachloropropene	H42	2163-80-6	MSMA	M355
1897-45-6	chlorothalonil	C286	2164-08-1	lenacil	L34
1912-24-9	atrazine	A252	2164-17-2	fluometuron	F47

2167-23-9	2,2-di(<i>tert</i> -butylperoxy)butane	D151	2432-99-7	11-aminoundecanoic acid	A155
2173-57-1	isobutyl 2-naphthyl ether	I94	2437-95-8	(±)- α -pinene	P197
2179-59-1	allyl propyl disulfide	A92	2438-88-2	2,3,5,6-tetrachloro-4-nitroanisole	T53
2186-24-5	4-cresyl glycidyl ether	C462	2439-01-2	quinomethionate	Q11
2210-79-9	2-cresyl glycidyl ether	C461	2439-10-3	dodine	D594
2212-67-1	molinate	M337	2439-99-8	glyphosine	G41
2223-82-7	neopentyl glycol diacrylate	N41	2465-27-2	auramine	A254
2223-93-0	cadmium stearate	C12	2471-92-3	1,3-dihydrobenzo[<i>c</i>]thiophene	D343
2224-15-9	ethylene glycol diglycidyl ether	E118	2475-45-8	C.I. Disperse Blue 1	C409
2227-13-6	tetrasul	T98	2489-77-2	trimethylthiourea	T326
2227-17-0	dienochlor	D277	2496-91-5	demeton-S sulfone	D56
2231-57-4	thiocarbazine	T124	2497-07-6	disulfoton sulfoxide	D567
2233-00-3	3,3,3-trichloro-1-propene	T266	2499-95-8	hexyl acrylate	H78
2234-13-1	octachloronaphthalene	O2	2524-03-0	dimethyl chlorothiophosphate	D407
2235-25-8	ethylmercury(II) phosphate	E144	2524-04-1	diethyl chlorothiophosphate	D300
2235-59-8	azoprocabazine	A272	2528-36-1	dibutyl phenyl phosphate	D159
2236-60-4	pterin	P345	2536-31-4	chlorflurenol-methyl	C129
2238-07-5	diglycidyl ether	D337	2540-82-1	formothion	F105
2243-27-8	octyl cyanide	O21	2551-62-4	sulfur hexafluoride	S151
2243-47-2	3-aminobiphenyl	A120	2570-26-5	pentadecylamine	P33
2243-62-1	1,5-naphthalenediamine	N10	2581-34-2	4-nitro- <i>m</i> -cresol	N105
2244-16-8	D-carvone	C93	2593-15-9	etridiazole	E185
2257-09-2	phenethyl isothiocyanate	P70	2595-54-2	mecarbam	M37
2274-67-1	dimethylvinphos	D460	2597-03-7	phenthoate	P89
2275-14-1	phenkapton	P77	2602-46-2	C.I. Direct Blue 6	C404
2275-18-5	prothoate	P342	2611-82-7	C.I. Acid Red 18	C394
2275-23-2	vamidothion	V9	2617-79-0	4-chloroformanilide	C202
2303-16-4	di-allate	D69	2631-37-0	promecarb	P286
2303-17-5	tri-allate	T198	2631-40-5	isoprocab	I116
2307-55-3	2,4-D, amine salt	D2	2634-33-5	1,2-benzisothiazolin-3-one	B54
2310-17-0	phosalone	P149	2636-26-2	cyanophos	C486
2312-35-8	propargite	P300	2642-71-9	azinphos-ethyl	A263
2314-09-2	flurenol-butyl	F85	2642-80-0	<i>p,p'</i> -DDMS	D32
2318-18-5	senkirkine	S23	2642-82-2	2,2-bis(4-chlorophenyl)ethanol	B126
2321-07-5	fluorescein	F51	2646-17-5	Oil Orange SS	O27
2338-37-6	levopropoxyphene	L39	2650-18-2	C.I. Acid Blue 9	C387
2353-45-9	C.I. Food Green 3	C412	2655-14-3	XMC	X4
2365-48-2	methyl mercaptoacetate	M248	2665-30-7	O-(4-nitrophenyl) O-phenyl	
2371-42-8	2-methylisoborneol	M240		methylphosphonothioate	N137
2381-21-7	1-methylpyrene	M294	2675-77-6	chloroneb	C219
2385-85-5	mirex	M334	2686-99-9	3,4,5-trimethacarb	T301
2387-23-7	<i>N,N'</i> -dicyclohexylurea	D270	2687-25-4	2,3-diaminotoluene	D86
2408-40-4	stilbestrol monoglucuronide	S118	2696-92-6	nitrosyl chloride	N177
2416-94-6	2,3,6-trimethylphenol	T321	2698-41-1	2-chlorobenzylidenemalononitrile	C175
2425-06-1	captafol	C58	2699-79-8	sulfuryl fluoride	S158
2425-10-7	xylylcarb	X16	2702-72-9	2,4-D, sodium salt	D16
2425-79-8	1,4-butanediol diglycidyl ether	B208	2703-13-1	O-ethyl O-[4-(methylthio)phenyl]	
2425-85-6	C.I. Pigment Red 3	C416		methylphosphonothioate	E150
2426-08-6	butyl glycidyl ether	B259	2705-87-5	allyl cyclohexylpropionate	A81
2429-74-5	C.I. Direct Blue 15	C405	2728-04-3	<i>N,N</i> -diethyl- <i>o</i> -toluamide	D320
2431-50-7	2,3,4-trichloro-1-butene	T244	2728-05-4	<i>N,N</i> -diethyl- <i>p</i> -toluamide	D321
2432-90-8	dilauryl phthalate	D364	2757-18-8	thallium(I) malonate	T105

2757-90-6	agaritine A59	3209-22-1	2,3-dichloronitrobenzene D227
2763-96-4	muscimol M356	3229-00-3	pentaerythrityl tetrabromide P37
2764-72-9	diquat D560	3244-90-4	tetrapropyl dithiopyrophosphate T96
2765-29-9	(<i>E,E,Z</i>)-1,5,9-cyclododecatriene C504	3248-28-0	dipropionyl peroxide D552
2778-04-3	endothion E24	3251-23-8	copper nitrate C438
2781-00-2	1,4-di(<i>tert</i> -butylperoxyisopropyl)benzene D154	3252-43-5	dibromoacetoneitrile D122
2782-57-2	dichlorocyanuric acid D202	3254-63-5	4-(methylthio)phenyl dimethyl phosphate M311
2783-94-0	C.I. Food Yellow 3 C415	3260-85-3	4-chloro-2-methylanisole C208
2797-51-5	quinoclamine Q8	3260-87-5	3-chloro- <i>o</i> -cresol C181
2807-30-9	2-propoxyethanol P316	3288-58-2	<i>O,O</i> -diethyl <i>S</i> -methyl dithiophosphate D310
2808-76-6	1,3-dimethylcyclohexene D410	3290-92-4	trimethylolpropane trimethacrylate T312
2809-21-4	etidronic acid E183	3296-90-0	dibromoneopentyl glycol D134
2813-95-8	dinoseb acetate D511	3320-83-0	2-chlorophenyl isocyanate C246
2832-19-1	2-chloro- <i>N</i> -(hydroxymethyl)acetamide C204	3337-71-1	asulam A251
2832-40-8	C.I. Disperse Yellow 3 C410	3347-22-6	dithianon D570
2835-39-4	allyl isovalerate A88	3351-28-8	1-methylchrysene M191
2855-13-2	isophorone diamine I111	3351-31-3	3-methylchrysene M193
2867-47-2	2-dimethylaminoethyl methacrylate D389	3351-32-4	2-methylchrysene M192
2885-00-9	1-octadecanethiol O3	3353-12-6	4-methylpyrene M296
2896-60-8	4-ethyl-1,3-benzenediol E98	3383-96-8	temephos T19
2909-38-8	3-chlorophenyl isocyanate C247	3389-71-7	1,2,3,4,7,7'-hexachloronorbornadiene H40
2921-88-2	chlorpyrifos C313	3391-86-4	1-octen-3-ol O18
2937-50-0	allyl chloroformate A79	3442-78-2	2-methylpyrene M295
2971-38-2	2,4-D, 4-chloro-2-butenyl ester D6	3452-09-3	1-nonyne N200
2971-90-6	clopidol C363	3454-07-7	4-ethylstyrene E171
2984-50-1	1,2-epoxyoctane E39	3458-22-8	improsulfan hydrochloride I16
3018-12-0	dichloroacetoneitrile D175	3458-28-4	D-mannose M30
3031-51-4	oxazolidinone hydrochloride O49	3486-35-9	zinc carbonate Z5
3034-19-3	2-nitrophenylhydrazine N135	3520-42-1	C.I. Acid Red 52 C396
3034-38-6	4-nitroimidazole N125	3542-36-7	dioctyltin dichloride D523
3037-72-7	(4-aminobutyl)diethoxymethylsilane A122	3546-10-9	phenesterine P65
3048-64-4	5-vinyl-2-norbornene V34	3564-09-8	C.I. Food Red 6 C414
3054-95-3	acrolein diethyl acetal A39	3567-69-9	C.I. Acid Red 14 C393
3060-89-7	metobromuron M322	3569-57-1	3-chloropropyl octyl sulfoxide C277
3068-88-0	β -butyrolactone B287	3570-75-0	nifurthiazole N59
3083-25-8	trichlorobutylene oxide T245	3599-32-4	Indocyanine Green I30
3087-16-9	C.I. Acid Green 50 C389	3614-30-0	emepronium bromide E16
3087-37-4	tetrapropyl orthotitanate T97	3615-37-0	D-fucose F114
3090-36-6	tributyltin laurate T217	3622-84-2	<i>N</i> -butylbenzenesulfonamide B248
3091-25-6	octyltin chloride O24	3625-06-7	mebeverine M35
3105-97-3	hycanthone H84	3634-67-1	chlorotrihexylsilane C303
3118-97-6	C.I. Solvent Orange 7 C420	3648-18-8	dioctyltin dilaurate D524
3120-74-9	3-methyl-4-(methylthio)phenol M254	3648-20-2	diundecyl phthalate D578
3129-91-7	dicyclohexylammonium nitrite D266	3648-21-3	diheptyl phthalate D340
3132-64-7	epibromohydrin E32	3688-53-7	furylamide F132
3164-29-2	ammonium tartrate A188	3689-24-5	sulfotep S147
3165-93-3	4-chloro- <i>o</i> -toluidine hydrochloride C295	3691-35-8	chlorophacinone C238
3173-53-3	cyclohexyl isocyanate C517	3697-24-3	5-methylchrysene M194
3173-72-6	naphthalene 1,5-diisocyanate N11	3697-27-6	5,6-dimethylchrysene D408
3178-22-1	1,1-dimethylethylcyclohexane D415	3724-65-0	crotonic acid C468

3734-95-0	cyanthoate C490	4680-78-8	C.I. Acid Green 3 C388
3734-97-2	amiton oxalate A157	4685-14-7	paraquat P11
3761-53-3	C.I. Acid Red 26 C395	4719-04-4	hexahydro-1,3,5-tris(2-hydroxyethyl)-s-triazine H51
3766-27-6	2,4-D, lithium salt D12		nitralin N64
3766-81-2	fenobucarb F12	4726-14-1	N-phenylphthalamic acid P130
3771-19-5	nafenopin N2	4727-29-1	isotretinoin I138
3778-73-2	ifosfamide I3	4759-48-2	2,3-dimethylindene D425
3811-04-9	potassium chlorate P242	4773-82-4	fluorosalan F72
3811-49-2	dioxabenzofos D527	4776-06-1	tributyltin phthalate T220
3813-05-6	benazolin B27	4782-29-0	tetrahydrofurfurylamine T75
3825-26-1	ammonium perfluorooctanoate A180	4795-29-3	1-hexen-3-ol H71
3844-45-9	C.I. Food Blue 2 C411	4798-44-1	tributyltin sulfide T222
3878-19-1	fuberidazole F113	4808-30-4	3-nitro-3-hexene N123
3883-43-0	<i>trans</i> -2,3-dichloro- <i>p</i> -dioxane D208	4812-22-0	bromophos-ethyl B184
3922-90-5	oleandomycin O29	4824-78-6	<i>N,N'</i> -dibutylhexamethylenediamine D146
3926-62-3	sodium chloroacetate S55	4835-11-4	karbutilate K4
3947-65-7	neomycin A N35	4849-32-5	vinburnine V22
3971-89-9	2,3,4-trimethacarb T300	4880-88-0	2,3,4,5-tetrachlorophenol T54
3982-91-0	thiophosphoryl chloride T141	4901-51-3	2-nitro- <i>m</i> -cresol N103
4016-14-2	glycidyl isopropyl ether G30	4920-77-8	pentaerythritol tetraacrylate P36
4044-65-9	bitoscanate B138	4986-89-4	benorylate B33
4067-16-7	pentaethylenehexamine P38	5003-48-5	C.I. Pigment Yellow 13 C419
4074-88-8	diethylene glycol diacrylate D302	5102-83-0	4,4'-methylenebis(cyclohexyl isocyanate) M211
4075-79-0	4-phenylacetanilide P90	5124-30-1	ditalimfos D569
4080-31-3	<i>N</i> -(3-chloroallyl)hexaminium chloride C153	5131-24-8	4-chloro- <i>m</i> -phenylenediamine C244
4097-36-3	dinosam D509	5131-60-2	1-butoxy-2-propanol B231
4098-71-9	isophorone diisocyanate I112	5131-66-8	D & C Red 9 D27
4101-68-2	1,10-dibromodecane D129	5160-02-1	3-chloro-2-methyl-1-butene C211
4104-14-7	phosacetim P148	5166-35-8	4-chlorobenzotrichloride C167
4106-66-5	3-dibenzofuranamine D114	5216-25-1	acrolein dibromide A38
4147-51-7	dipropetryn D551	5221-17-0	dimethirimol D375
4151-50-2	sulfluramid S142	5221-53-4	carboxin C84
4164-28-7	dimethylnitramine D443	5234-68-4	flucloxacillin F41
4230-97-1	allyl octanoate A89	5250-39-5	glycidyl 4-nitrophenyl ether G33
4234-79-1	kelevan K6	5255-75-4	oxycarboxin O56
4301-50-2	fluenetil F44	5259-88-1	piprotal P207
4316-42-1	<i>N</i> -butylimidazole B263	5281-13-0	nonyltrichlorosilane N199
4342-03-4	dacarbazine D17	5283-67-0	β-ecdysterone E1
4342-36-3	tributyltin benzoate T214	5289-74-7	5-chloro- <i>o</i> -cresol C185
4376-20-9	mono(2-ethylhexyl) phthalate M344	5306-98-9	2-nitro- <i>p</i> -phenylenediamine N133
4418-26-2	sodium dehydroacetate S60	5307-14-2	2,6-dibromo-4-chlorophenol D127
4418-66-0	6,6'-thiobis(4-chloro- <i>o</i> -cresol) T120	5324-13-0	sulfamic acid S137
4461-41-0	2-chloro-2-butene C177	5329-14-6	1-undecanethiol U3
4461-48-7	4-methyl-2-pentene M285	5332-52-5	(2-chlorophenyl)thiourea C251
4464-23-7	cadmium formate C9	5344-82-1	3-chloro- <i>p</i> -anisidine C158
4465-94-5	cytoxal alcohol cyclohexylammonium salt C548	5345-54-0	<i>N</i> -nitrosodi- <i>sec</i> -butylamine N147
4466-14-2	jasmolin I J1	5350-17-4	citral C351
4549-40-0	<i>N</i> -nitroso- <i>N</i> -methylvinylamine N165	5392-40-5	monooctyl phthalate M346
4644-96-6	tributyltin succinate T221	5393-19-1	triisopropyl borate T298
4658-28-0	aziprotryne A265	5419-55-6	2-phenyl-1,3-dithiane P99
		5425-44-5	

5428-54-6	5-nitro- <i>o</i> -cresol	N106	6731-36-8	1,1-bis(<i>tert</i> -butylperoxy)-3,3,5-trimethylcyclohexane	B117
5431-33-4	glycidyl oleate	G34	6795-23-9	aflatoxin M ₁	A57
5437-45-6	benzyl bromoacetate	B93	6846-50-0	2,2,4-trimethyl-1,3-pentanediol diisobutyrate	T316
5456-28-0	selenium diethyldithiocarbamate	S15	6872-06-6	2-methylindoline	M239
5522-43-0	1-nitropyrene	N141	6915-15-7	malic acid	M15
5543-58-8	(+)-warfarin	W2	6917-35-7	inositol	I37
5598-13-0	chlorpyrifos-methyl	C314	6923-22-4	monocrotophos	M343
5609-19-8	3,4,5-trichlorophenol	T260	6938-94-9	diisopropyl adipate	D357
5707-69-7	drazoxolon	D600	6959-47-3	2-picoyl chloride hydrochloride	P186
5714-22-7	disulfur decafluoride	D568	6980-18-3	kasugamycin	K5
5725-91-7	7-ethoxyresorufin	E86	6988-21-2	dioxacarb	D528
5798-79-8	α -bromobenzyl cyanide	B162	7005-72-3	4-chlorophenyl phenyl ether	C250
5825-87-6	3-CPA	C451	7008-42-6	acronycine	A40
5834-96-8	azothoate	A273	7023-61-2	C.I. Pigment Red 48:2	C418
5836-10-2	chloropropylate	C276	7164-98-9	1-phenylimidazole	P111
5836-29-3	coumatetralyl	C448	7166-19-0	β -bromo- β -nitrostyrene	B182
5878-19-3	methoxyacetone	M131	7173-51-5	didecyldimethylammonium chloride	D274
5891-21-4	5-chloro-2-pentanone	C236	7220-81-7	aflatoxin B ₂	A54
5902-51-2	terbacil	T20	7235-40-7	β -carotene	C89
5910-89-4	2,3-dimethylpyrazine	D451	7241-98-7	aflatoxin G ₂	A56
5915-41-3	terbuthylazine	T24	7267-14-3	4,5-dichloronaphthalene-1,8-dicarboxylic anhydride	D226
5965-66-2	β -lactose	L3	7287-19-6	prometryn	P289
5970-32-1	mercury salicylate	M84	7287-36-7	monalide	M340
5972-73-6	ammonium oxalate	A179	7292-16-2	propaphos	P298
5989-27-5	(<i>R</i>)-(+)-limonene	L46	7320-37-8	1,2-epoxyhexadecane	E37
6051-87-2	β -naphthoflavone	N14	7379-51-3	3,5-dimethyl-4-(methylthio)phenol	D431
6108-10-7	ϵ -lindane	L48	7414-83-7	disodium etidronate	D562
6117-91-5	crotyl alcohol	C470	7421-93-4	endrin aldehyde	E26
6130-75-2	2,4,5-trichloroanisole	T238	7429-90-5	aluminium	A96
6146-52-7	5-nitroindole	N126	7429-91-6	dysprosium	D604
6164-98-3	chlordimeform	C121	7439-88-5	iridium	I64
6202-15-9	1,2,3,4-tetranitrocarbazole	T94	7439-89-6	iron	I66
6358-29-8	C.I. Direct Red 39	C408	7439-91-0	lanthanum	L4
6358-53-8	C.I. Solvent Red 80	C423	7439-92-1	lead	L11
6358-64-1	4-chloro-2,5-dimethoxyaniline	C193	7439-93-2	lithium	L52
6358-85-6	Diarylanilide Yellow	D96	7439-94-3	lutetium	L60
6369-59-1	2,5-toluenediamine sulfate	T174	7439-96-5	manganese	M22
6373-74-6	C.I. Acid Orange 3	C390	7439-97-6	mercury	M64
6385-58-6	sodium bithionolate	S49	7439-98-7	molybdenum	M338
6423-43-4	propylene glycol dinitrate	P329	7440-00-8	neodymium	N33
6440-58-0	<i>N,N'</i> -dimethylol-5,5-dimethylhydantoin	D446	7440-02-0	nickel	N44
6443-92-1	(<i>Z</i>)-2-heptene	H27	7440-03-1	niobium	N61
6452-71-7	oxprenolol	O52	7440-04-2	osmium	O37
6459-94-5	C.I. Acid Red 114	C398	7440-06-4	platinum	P212
6471-49-4	C.I. Pigment Red 23	C417	7440-09-7	potassium	P237
6484-52-2	ammonium nitrate	A178	7440-10-0	praseodymium	P268
6533-73-9	thallium(I) carbonate	T102	7440-15-5	rhenium	R8
6556-11-2	inositol niacinate	I38	7440-16-6	rhodium	R10
6575-00-4	3,5-dichlorobenzonitrile	D196			
6616-80-4	eglinazine-ethyl	E12			
6639-30-1	2,4,5-trichlorotoluene	T268			

7440-17-7	rubidium	R19	7488-99-5	α -carotene	C88
7440-18-8	ruthenium	R21	7493-74-5	allyl phenoxyacetate	A90
7440-19-9	samarium	S7	7496-02-8	6-nitrochrysene	N102
7440-21-3	silicon	S30	7525-62-4	3-ethylstyrene	E170
7440-22-4	silver	S33	7542-37-2	neomycin E	N38
7440-23-5	sodium	S39	7546-30-7	mercury(II) chloride	M70
7440-24-6	strontium	S121	7550-45-0	titanium tetrachloride	T166
7440-25-7	tantalum	T7	7553-56-2	iodine	I40
7440-27-9	terbium	T21	7558-79-4	sodium monohydrogen phosphate	S79
7440-28-0	thallium	T100	7572-29-4	dichloroacetylene	D177
7440-29-1	thorium	T148	7580-67-8	lithium hydride	L54
7440-31-5	tin	T158	7585-39-9	β -cyclodextrin	C501
7440-32-6	titanium	T164	7601-54-9	trisodium phosphate	T359
7440-33-7	tungsten	T371	7601-89-0	sodium perchlorate	S83
7440-36-0	antimony	A221	7601-90-3	perchloric acid	P52
7440-38-2	arsenic	A240	7616-94-6	perchloryl fluoride	P53
7440-39-3	barium	B5	7631-86-9	silica	S29
7440-41-7	beryllium	B102	7631-89-2	sodium arsenate	S44
7440-43-9	cadmium	C2	7631-90-5	sodium bisulfite	S48
7440-45-1	cerium	C101	7631-99-4	sodium nitrate	S80
7440-46-2	caesium	C16	7632-00-0	sodium nitrite	S81
7440-47-3	chromium	C329	7632-51-1	vanadium tetrachloride	V13
7440-48-4	cobalt	C369	7637-07-2	boron trifluoride	B147
7440-50-8	copper	C429	7642-10-6	(Z)-3-heptene	H28
7440-53-1	europium	E189	7646-69-7	sodium hydride	S70
7440-54-2	gadolinium	G1	7646-78-8	tin(IV) chloride	T160
7440-55-3	gallium	G3	7646-79-9	cobalt(II) chloride	C372
7440-57-5	gold	G42	7646-85-7	zinc chloride	Z6
7440-58-6	hafnium	H1	7646-93-7	potassium hydrogen sulfate	P253
7440-59-7	helium	H11	7647-01-0	hydrogen chloride	H99
7440-60-0	holmium	H83	7647-10-1	palladium chloride	P2
7440-61-1	uranium	U9	7647-18-9	antimony pentachloride	A223
7440-62-2	vanadium	V10	7647-19-0	phosphorus pentafluoride	P161
7440-65-5	yttrium	Y2	7659-86-1	2-ethylhexyl mercaptoacetate	E134
7440-66-6	zinc	Z2	7659-95-2	betanin	B107
7440-67-7	zirconium	Z20	7661-55-4	5-methylquinoline	M300
7440-68-8	astatine	A250	7664-38-2	phosphoric acid	P156
7440-70-2	calcium	C21	7664-39-3	hydrogen fluoride	H101
7440-73-5	francium	F110	7664-41-7	ammonia	A161
7440-74-6	indium	I27	7664-93-9	sulfuric acid	S152
7446-08-4	selenium dioxide	S16	7665-72-7	<i>tert</i> -butyl glycidyl ether	B260
7446-09-5	sulfur dioxide	S150	7673-09-8	trichloromelamine	T251
7446-11-9	sulfur trioxide	S157	7681-11-0	potassium iodide	P256
7446-14-2	lead sulfate	L30	7681-49-4	sodium fluoride	S66
7446-18-6	thallium(I) sulfate	T108	7681-52-9	sodium hypochlorite	S74
7446-27-7	lead phosphate	L27	7681-57-4	sodium metabisulfite	S78
7446-34-6	selenium sulfide	S20	7681-93-8	pimaricin	P191
7446-70-0	aluminium chloride	A99	7696-12-0	tetramethrin	T85
7447-39-4	copper(II) chloride	C434	7697-37-2	nitric acid	N68
7447-40-7	potassium chloride	P243	7699-45-8	zinc bromide	Z4
7487-94-7	mercury(II) chloride	M71	7700-17-6	α -methylbenzyl 3-hydroxycrotonate, dimethyl phosphate	M167
7488-56-4	selenium disulfide	S17			

7704-34-9	sulfur S149	7779-88-6	zinc nitrate Z11
7704-99-6	zirconium hydride Z21	7781-98-8	ethyl 3-hydroxybenzoate E137
7705-07-9	titanium trichloride T167	7782-39-0	deuterium D61
7705-08-0	iron(III) chloride I69	7782-41-4	fluorine F52
7718-54-9	nickel chloride N46	7782-42-5	graphite G45
7718-98-1	vanadium trichloride V14	7782-44-7	oxygen O60
7719-09-7	thionyl chloride T136	7782-49-2	selenium S14
7719-12-2	phosphorus trichloride P166	7782-50-5	chlorine C135
7720-78-7	iron(II) sulfate I76	7782-65-2	germanium tetrahydride G13
7722-64-7	potassium permanganate P260	7782-79-8	hydrogen azide H97
7722-84-1	hydrogen peroxide H103	7782-92-5	sodium amide S41
7722-88-5	sodium pyrophosphate S88	7782-99-2	sulfurous acid S155
7723-14-0	phosphorus P158	7783-00-8	selenious acid S13
7726-95-6	bromine B154	7783-06-4	hydrogen sulfide H105
7727-15-3	aluminium bromide A97	7783-07-5	hydrogen selenide H104
7727-18-6	vanadium oxytrichloride V11	7783-08-6	selenic acid S12
7727-21-1	potassium persulfate P261	7783-18-8	ammonium thiosulfate A191
7727-37-9	nitrogen N119	7783-20-2	ammonium sulfate A185
7727-43-7	barium sulfate B24	7783-30-4	mercury(I) iodide M75
7727-54-0	ammonium peroxydisulfate A181	7783-33-7	potassium tetraiodomercurate(II) P266
7733-02-0	zinc sulfate Z17	7783-35-9	mercury(II) sulfate M86
7738-94-5	chromic acid C328	7783-36-0	mercury(I) sulfate M85
7757-79-1	potassium nitrate P257	7783-41-7	oxygen difluoride O61
7757-81-5	sodium sorbate S91	7783-46-2	lead fluoride L22
7757-82-6	sodium sulfate S92	7783-47-3	tin(II) fluoride T161
7757-83-7	sodium sulfite S94	7783-50-8	iron(III) fluoride I71
7758-01-2	potassium bromate P241	7783-54-2	nitrogen trifluoride N121
7758-05-6	potassium iodate P255	7783-56-4	antimony trifluoride A226
7758-09-0	potassium nitrite P258	7783-60-0	sulfur tetrafluoride S156
7758-19-2	sodium chlorite S54	7783-70-2	antimony pentafluoride A224
7758-29-4	sodium triphosphate S98	7783-79-1	selenium hexafluoride S18
7758-87-4	calcium phosphate C40	7783-80-4	tellurium hexafluoride T17
7758-89-6	copper(I) chloride C433	7783-82-6	tungsten hexafluoride T373
7758-94-3	iron(II) chloride I68	7784-08-9	silver arsenite S34
7758-95-4	lead chloride L15	7784-21-6	aluminium hydride A100
7758-97-6	lead chromate L16	7784-27-2	aluminium nitrate nonahydrate A102
7758-98-7	copper sulfate C442	7784-34-1	arsenic trichloride A243
7761-88-8	silver nitrate S36	7784-40-9	lead arsenate L13
7772-99-8	tin(II) chloride T159	7784-41-0	potassium arsenate P238
7773-06-0	ammonium sulfamate A184	7784-42-1	arsine A246
7774-29-0	mercury(II) iodide M76	7784-44-3	ammonium arsenate A163
7775-09-9	sodium chlorate S53	7784-46-5	sodium arsenite S45
7775-11-3	sodium chromate S56	7785-26-4	(1S)-(-)- α -pinene P194
7775-27-1	sodium persulfate S84	7785-70-8	(1R)-(+)- α -pinene P196
7778-18-9	calcium sulfate C44	7786-34-7	mevinphos M330
7778-39-4	arsenic acid A241	7786-81-4	nickel sulfate N50
7778-44-1	calcium arsenate C22	7787-36-2	barium permanganate B16
7778-50-9	potassium dichromate P246	7787-47-5	beryllium chloride B103
7778-54-3	calcium hypochlorite C34	7787-49-7	beryllium fluoride B104
7778-74-7	potassium perchlorate P259	7787-71-5	bromine trifluoride B157
7778-80-5	potassium sulfate P264	7788-97-8	chromium(III) fluoride C335
7779-27-3	1,3,5-triethylhexahydro-s-triazine T285	7788-98-9	ammonium chromate A171

7789-00-6	potassium chromate P244	8022-00-2	demeton-methyl D50
7789-06-2	strontium chromate S122	8023-53-8	<i>N</i> -alkyl(C ₈ -C ₁₈)dimethyl-3, 4-
7789-09-5	ammonium dichromate A172		dichlorobenzylammonium chloride A67
7789-12-0	sodium dichromate dihydrate S62	8030-30-6	naphtha N5
7789-18-6	caesium nitrate C18	8050-88-2	celluloid C96
7789-21-1	fluorosulfonic acid F75	8052-16-2	actinomycin C A45
7789-23-3	potassium fluoride P248	8052-41-3	Stoddard solvent S119
7789-29-9	potassium hydrogen fluoride P252	8052-42-4	asphalt, fumes A249
7789-30-2	bromine pentafluoride B156	8056-92-6	ovulen O41
7789-38-0	sodium bromate S51	8065-48-3	demeton D49
7789-42-6	cadmium bromide C4	8068-05-1	lignin alkali L42
7789-43-7	cobalt(II) bromide C370	9000-01-5	Gum Arabic G53
7789-47-1	mercury(II) bromide M69	9000-07-1	carrageenan C91
7789-60-8	phosphorus tribromide P165	9000-30-0	Guar Gum G51
7789-89-1	1,1,1-trichloropropane T262	9000-36-6	karaya gum K3
7790-79-6	cadmium fluoride C7	9000-40-2	locust bean gum L57
7790-80-9	cadmium iodide C10	9001-62-1	lipase L51
7790-91-2	chlorine trifluoride C138	9001-73-4	papain P3
7790-94-5	chlorosulfonic acid C285	9002-18-0	agar A58
7790-99-0	iodine monochloride I41	9002-84-0	polytetrafluoroethylene P232
7791-12-0	thallium(I) chloride T103	9002-86-2	polyvinyl chloride P235
7791-23-3	selenium oxychloride S19	9002-88-4	polyethylene P224
7803-49-8	hydroxylamine H112	9002-89-5	polyvinyl alcohol P234
7803-51-2	phosphine P155	9002-93-1	octoxynol O20
7803-55-6	ammonium metavanadate A177	9003-11-6	poloxamer P218
7803-62-5	silane S28	9003-20-7	polyvinyl acetate P233
8000-41-7	terpineol T35	9003-39-8	polyvinylpyrrolidone P236
8001-35-2	camphenchlor C48	9003-53-6	polystyrene P231
8001-50-1	polychloroterpenes P221	9004-34-6	cellulose C97
8001-54-5	benzalkonium chloride B41	9004-66-4	iron(III) dextran I70
8001-58-9	creosote C453	9004-67-5	methylcellulose M185
8001-79-4	castor oil C94	9004-70-0	cellulose nitrate C98
8002-16-2	rosin oil R17	9005-25-8	starch S110
8002-74-2	paraffin wax P7	9005-64-5	polysorbate 20 P227
8003-05-2	phenylmercuric nitrate, basic P120	9005-65-6	polysorbate 80 P230
8003-19-8	D-D D28	9005-66-7	polysorbate 40 P228
8003-22-3	C.I. Solvent Yellow 33 C427	9005-67-8	polysorbate 60 P229
8003-34-7	pyrethrum P354	9006-42-2	metiram M321
8004-92-0	Quinoline Yellow Q10	9009-86-3	ricin R13
8005-03-6	C.I. Acid Black 2 C385	9011-14-7	polymethyl methacrylate P226
8006-61-9	gasoline, natural G8	9016-00-6	polydimethylsiloxane P222
8006-64-2	turpentine oil T374	9016-00-6	dimethicone D373
8007-45-2	coal tar C366	9016-87-9	phenyl isocyanate formaldehyde polymer P114
8008-20-6	kerosene K7		
8011-63-0	Bordeaux mixture B142	9080-17-5	ammonium polysulfide A183
8012-95-1	mineral oil M333	10004-44-1	hymexazol H121
8012-96-2	ipecacuanha I60	10016-20-3	α -cyclodextrin C500
8014-95-7	sulfuric acid (fuming) S153	10022-31-8	barium nitrate B13
8015-12-1	Norlestrin N207	10022-70-5	sodium hypochlorite pentahydrate S75
8015-30-3	Enovid E28	10024-97-2	nitrous oxide N183
8015-86-9	carnauba wax C87	10025-65-7	platinum dichloride P213
8018-01-7	mancozeb M19	10025-67-9	sulfur monochloride S154

10025-73-7	chromium(III) chloride	C334	10124-50-2	potassium arsenite	P239
10025-78-2	trichlorosilane	T267	10124-56-8	sodium hexametaphosphate	S69
10025-82-8	indium trichloride	I29	10137-69-6	3-cyclohexenyltrichlorosilane	C512
10025-87-3	phosphorus oxychloride	P159	10137-74-3	calcium chlorate	C26
10025-91-9	antimony trichloride	A225	10163-15-2	disodium fluorophosphate	D563
10025-97-5	iridium tetrachloride	I65	10192-30-0	ammonium bisulfite	A166
10026-01-4	osmium tetrachloride	O38	10196-04-0	ammonium sulfite	A187
10026-07-0	tellurium tetrachloride	T18	10210-68-1	cobalt carbonyl	C371
10026-08-1	thorium chloride	T149	10217-52-4	hydrazine hydrate	H88
10026-11-6	zirconium tetrachloride	Z24	10222-01-2	2,2-dibromo-3-nitrilopropionamide	D135
10026-13-8	phosphorus pentachloride	P160	10265-92-6	methamidophos	M111
10028-15-6	ozone	O65	10294-33-4	boron tribromide	B145
10028-22-5	iron(III) sulfate	I77	10294-34-5	boron trichloride	B146
10031-13-7	lead arsenite	L14	10294-56-1	phosphorous acid	P157
10031-18-2	mercury(I) bromide	M68	10311-84-9	dialifos	D68
10031-59-1	thallium hydrogen sulfate	T104	10326-21-3	magnesium chlorate	M3
10034-81-8	magnesium perchlorate	M7	10361-37-2	barium chloride	B11
10034-85-2	hydrogen iodide	H102	10361-92-9	yttrium chloride	Y3
10034-93-2	hydrazine sulfate	H89	10361-93-0	yttrium nitrate	Y4
10035-10-6	hydrogen bromide	H98	10377-60-3	magnesium nitrate	M5
10042-76-9	strontium nitrate	S123	10377-66-9	manganese nitrate	M26
10043-01-3	aluminium sulfate	A107	10380-28-6	oxine-copper	O50
10043-67-1	aluminium potassium sulfate	A105	10380-29-7	copper sulfate, ammoniated	C443
10043-92-2	radon	R1	10415-75-5	mercury(I) nitrate	M77
10045-89-3	iron(II) ammonium sulfate	I67	10421-48-4	iron(III) nitrate	I73
10045-94-0	mercury(II) nitrate	M78	10436-39-2	1,1,2,3-tetrachloropropene	T59
10048-13-2	sterigmatocystin	S114	10453-86-8	resmethrin	R4
10048-32-5	parascorbic acid	P12	10476-95-6	methacrolein diacetate	M104
10049-04-4	chlorine dioxide	C136	10482-56-1	α -terpineol	T36
10049-05-5	chromium(II) chloride	C333	10540-29-1	tamoxifen	T5
10049-07-7	rhodium trichloride	R11	10544-72-6	dinitrogen tetroxide	D478
10099-58-8	lanthanum trichloride	L5	10544-73-7	dinitrogen trioxide	D479
10099-74-8	lead nitrate	L25	10552-74-6	nitrothal-isopropyl	N178
10101-41-4	calcium sulfate dihydrate	C45	10553-31-8	barium bromide	B8
10101-53-8	chromium(III) sulfate	C338	10588-01-9	sodium dichromate	S61
10101-63-0	lead iodide	L24	10589-74-9	1-amy1-1-nitroso-urea	A203
10101-89-0	trisodium phosphate dodecahydrate	T360	10595-95-6	<i>N</i> -nitroso- <i>N</i> -methylethylamine	N161
10102-03-1	dinitrogen pentoxide	D477	10599-90-3	chloramine	C112
10102-06-4	uranyl nitrate	U11	10605-21-7	carbendazim	C65
10102-18-8	sodium selenite	S90	11003-45-5	chlorophyll c	C255
10102-20-2	sodium tellurite	S95	11041-12-6	cholestyramine	C325
10102-43-9	nitric oxide	N69	11056-06-7	bleomycin	B140
10102-44-0	nitrogen dioxide	N120	11096-18-7	cufraneb	C473
10102-45-1	thallium(I) nitrate	T106	11096-82-5	Aroclor 1260	A239
10103-50-1	magnesium arsenate	M2	11097-69-1	Aroclor 1254	A238
10108-64-2	cadmium chloride	C5	11103-57-4	vitamin A	V40
10112-91-1	calomel	C47	11104-28-2	Aroclor 1221	A234
10118-76-0	calcium permanganate	C38	11141-16-5	Aroclor 1232	A235
10124-36-4	cadmium sulfate	C13	11141-17-6	azadirachtin	A258
10124-37-5	calcium nitrate	C36	12001-28-4	crocidolite	C465
10124-43-3	cobalt(II) sulfate	C379	12001-29-5	chrysotile	C342
10124-48-8	mercury ammonium chloride	M66	12002-03-8	Paris Green	P15

12002-19-6	mercury nucleate M79	13181-17-4	bromofenoxim B176
12002-48-1	trichlorobenzene (technical mixture) T240	13194-48-4	ethoprophos E74
12024-21-4	gallium oxide G6	13256-11-6	<i>N</i> -nitroso- <i>N</i> -(2-phenylethyl)methylamine N171
12030-88-5	potassium superoxide P265		
12035-72-2	nickel subsulfide N49	13256-22-9	<i>N</i> -nitrososarcosine N175
12044-79-0	arsenic disulfide A242	13292-46-1	rifampicin R15
12054-48-7	nickel hydroxide N47	13347-42-7	4-chloro-2-cyclopentylphenol C189
12057-74-8	magnesium phosphide M8	13351-73-0	1-methylbenzotriazole M163
12058-85-4	sodium phosphide S87	13356-08-6	fenbutatin oxide F7
12070-12-1	tungsten carbide T372	13360-45-7	chlorbromuron C116
12071-83-9	propineb P307	13360-57-1	dimethylaminosulfonyl chloride D393
12079-65-1	manganese cyclopentadienyl tricarbonyl M23	13360-64-0	2-ethyl-5-methylpyrazine E149
		13366-73-9	photodieldrin P168
12108-13-3	manganese 2-methylcyclopentadienyl tricarbonyl M25	13410-01-0	sodium selenate S89
		13417-43-1	1-chloro-2-methyl-2-butene C210
12116-66-4	hafnocene dichloride H3	13426-91-0	cupriethylenediamine C477
12122-67-7	zineb Z18	13450-90-3	gallium trichloride G7
12125-01-8	ammonium fluoride A173	13453-07-1	gold trichloride G43
12125-02-9	ammonium chloride A169	13454-96-1	platinum tetrachloride P214
12135-76-1	ammonium sulfide A186	13457-18-6	pyrazophos P350
12141-20-7	lead phosphite dibasic L28	13463-39-3	nickel tetracarbonyl N51
12192-57-3	aurothioglucose A255	13463-40-6	iron pentacarbonyl I75
12230-99-8	barium polysulfides (BaS ₂) B18	13463-41-7	zinc pyrithione Z15
12231-01-5	barium polysulfides (BaS ₃) B19	13463-67-7	titanium dioxide T165
12259-92-6	ammonium polysulfide A183	13465-95-7	barium perchlorate B15
12304-65-3	hydrotalcite H108	13472-45-2	sodium tungstate S99
12310-22-4	copper acetoarsenite C431	13477-00-4	barium chlorate B10
12427-38-2	maneb M21	13494-80-9	tellurium T16
12448-67-8	barium polysulfides (BaS ₄) B20	13494-90-1	gallium nitrate G5
12448-68-9	barium polysulfides (BaS ₅) B21	13499-05-3	hafnium chloride H2
12504-13-1	strontium phosphide S124	13510-49-1	beryllium sulfate B106
12519-36-7	EDTA zinc salt E10	13516-27-3	iminocytidine I10
12653-71-3	mercury(II) oxide M81	13530-65-9	zinc chromate Z7
12672-29-6	Aroclor 1248 A237	13537-32-1	fluorophosphoric acid F71
12674-11-2	Aroclor 1016 A233	13548-38-4	chromium(III) nitrate C336
12771-68-5	ancymidol A207	13551-87-6	misonidazole M335
12788-93-1	butyl acid phosphate B237	13552-44-8	4,4'-methylenedianiline dihydrochloride M219
13010-07-6	1-propyl-3-nitro-3-nitrosoguanidine P335		
13010-47-4	lomustine L58	13593-03-8	quinalphos Q5
13014-18-1	2,4-dichlorobenzotrithioride D197	13597-99-4	beryllium nitrate B105
13048-33-4	1,6-hexanediol diacrylate H61	13637-63-3	chlorine pentafluoride C137
13071-79-9	terbufos T22	13637-76-8	lead perchlorate L26
13073-29-5	6-nitro- <i>o</i> -cresol N108	13674-87-8	tris(1,3-dichloro-2-propyl) phosphate T353
13108-52-6	2,3,5,6-tetrachloro-4-(methylsulfonyl)pyridine T52	13684-56-5	desmedipham D59
		13684-63-4	phenmedipham P78
13116-53-5	1,2,2,3-tetrachloropropane T58	13743-07-2	1-(2-hydroxyethyl)-1-nitrosourea H111
13121-70-5	cyhexatin C535	13746-89-9	zirconium nitrate Z22
13122-18-4	<i>tert</i> -butyl peroxy-3,5,5-trimethylhexanoate B274	13765-19-0	calcium chromate C28
		13814-96-5	lead fluoborate L21
13138-45-9	nickel nitrate N48	13823-29-5	thorium nitrate T151
13149-00-3	<i>cis</i> -hexahydrophthalic anhydride H50	13826-83-0	ammonium tetrafluoroborate A189
13171-21-6	phosphamidon P154	13838-16-9	enflurane E27

13840-33-0	lithium hypochlorite	L55	15972-60-8	alachlor	A60
13863-41-7	bromine chloride	B155	16065-83-1	chromium(III)	C330
13952-84-6	<i>sec</i> -butylamine	B240	16071-86-6	C.I. Direct Brown 95	C407
13962-39-5	chlorophyllin b	C258	16091-18-2	dioctyltin maleate	D525
13967-90-3	barium bromate	B7	16111-62-9	di- <i>sec</i> -octyl peroxydicarbonate	D517
13987-01-4	tripropylene	T343	16118-49-3	carbetamide	C66
14017-41-5	cobalt(II) sulfamate	C378	16136-84-8	(Z)-1-chloropropene	C270
14214-32-5	difenoxuron	D324	16136-85-9	(E)-1-chloropropene	C269
14255-88-0	fenazaflor	F5	16215-49-9	dibutyl peroxydicarbonate	D152
14324-55-1	zinc diethyldithiocarbamate	Z9	16219-75-3	5-ethylidene-2-norbornene	E138
14362-31-3	chlorocyclizine hydrochloride	C188	16543-55-8	<i>N</i> -nitrosornicotine	N169
14437-17-3	chlorfenprop-methyl	C126	16568-02-8	acetaldehyde formylmethylhydrazone	A8
14459-29-1	hematoporphyrin	H13	16672-87-0	ethephon	E63
14464-46-1	cristobalite	C464	16714-68-4	1,1,2,2,3-pentachloropropane	P31
14484-64-1	ferbam	F30	16721-80-5	sodium hydrosulfide	S72
14542-23-5	fluorspar	F80	16752-77-5	methomyl	M126
14644-61-2	zirconium(IV) sulfate	Z23	16813-36-8	1-nitroso-5,6-dihydrouacil	N150
14674-72-7	calcium chlorite	C27	16842-03-8	cobalt hydrocarbonyl	C374
14721-21-2	copper chlorate	C432	16853-85-3	lithium aluminium hydride	L53
14807-96-6	talca	T3	16871-90-2	potassium fluorosilicate	P250
14808-60-7	quartz	Q1	16872-11-0	fluoboric acid	F46
14816-18-3	phoxim	P170	16893-85-9	sodium fluorosilicate	S68
14901-07-6	β -ionone	I58	16919-19-0	ammonium fluorosilicate	A174
14901-08-7	cycasin	C494	16919-58-7	ammonium chloroplatinate(IV)	A170
14977-61-8	chromyl chloride	C339	16923-95-8	potassium fluorozirconate(IV)	P251
15096-52-3	cryolite	C472	16940-66-2	sodium borohydride	S50
15104-61-7	1,1,2,3,3-pentachloropropane	P32	16941-12-1	chloroplatinic acid	C261
15258-73-8	2,6-dichlorobenzyl alcohol	D198	16949-65-8	magnesium fluorosilicate	M4
15263-52-2	cartap hydrochloride	C92	16961-83-4	fluorosilicic acid	F74
15299-99-7	napropamide	N28	17010-21-8	cadmium fluorosilicate	C8
15310-01-7	benodanil	B31	17040-19-6	demeton-S-methyl sulfone	D55
15356-70-4	DL-menthol	M54	17084-08-1	fluorosilicate	F73
15468-32-3	tridymite	T274	17092-92-1	dihydroactinidolide	D342
15481-70-6	2,6-diaminotoluene dihydrochloride	D91	17109-49-8	edifenphos	E2
15489-90-4	hematin	H12	17140-78-2	propoxyphene napsylate	P320
15506-53-3	cyclobutane-1,3-dione	C499	17372-87-1	eosin	E29
15512-36-4	calcium dithionite	C31	17465-86-0	γ -cyclodextrin	C502
15545-48-9	chlorotoluron	C298	17606-31-4	bensultap	B37
15557-00-3	3-chloro-4-diethylaminobenzenediazonium trichlorozincate	C190	17617-23-1	flurazepam	F84
15571-58-1	dioctyltin bis(2-ethylhexyl thioglycolate)	D521	17639-93-9	methyl 2-chloropropionate	M189
15611-43-5	chlorophyllin a	C257	17673-25-5	phorbol	P146
15625-89-5	trimethylolpropane triacrylate	T311	17702-41-9	decaborane	D37
15663-27-1	cisplatin	C350	17702-57-7	formparanate	F106
15686-71-2	cephalexin	C100	17804-35-2	benomyl	B32
15687-27-1	ibuprofen	I2	17902-23-7	furaflour	F118
15699-18-0	nickel ammonium sulfate	N45	17924-92-4	zearelenone	Z1
15826-37-6	sodium chromoglycate	S57	18172-67-3	(1S)-(-)- β -pinene	P199
15829-53-5	mercury(I) oxide	M81	18181-70-9	iodofenphos	I50
15879-93-3	chloralose	C109	18181-80-1	bromopropylate	B187
15950-66-0	2,3,4-trichlorophenol	T255	18250-63-0	dimethyl (Z)-1-methyl-2-dimethylcarbamoylviny phosphate	D428
			18323-44-9	clindamycin	C354

18540-29-9	chromium(vi) C331	22224-92-6	fenamiphos F3
18559-94-9	salbutamol S3	22248-79-9	tetrachlorvinphos T60
18662-53-8	trisodium nitrilotriacetate, monohydrate T358	22259-30-9	formetanate F102
18691-97-9	methabenzthiazuron M101	22398-80-7	indium phosphide I28
18708-70-8	2,4,6-trichloronitrobenzene T254	22494-42-4	diflunisal D328
18854-01-8	isoxathion I143	22750-93-2	ethyl perchlorate E159
18883-66-4	streptozocin S120	22781-23-3	bendiocarb B28
19010-66-3	lead dimethyldithiocarbamate L18	22898-01-7	flupropanate-sodium F83
19044-88-3	oryzalin O36	22916-47-8	miconazole M332
19287-45-7	diborane D121	22936-75-0	dimethametryn D372
19408-74-3	1,2,3,7,8,9-hexachlorodibenzo- <i>p</i> -dioxin H37	22966-79-6	estradiol mustard E52
19429-30-2	di- <i>tert</i> -butyltin dichloride D162	22967-92-6	methylmercury M249
19485-03-1	1,3-butanediol diacrylate B206	23031-36-9	prallethrin P267
19624-22-7	pentaborane(9) P23	23103-98-2	pirimicarb P208
19666-30-9	oxadiazon O44	23135-22-0	oxamyl O47
19700-21-1	geosmin G11	23184-66-9	butachlor B196
19834-02-7	cyclohexylamine sulfate C515	23214-92-8	doxorubicin D596
19910-65-7	di- <i>sec</i> -butyl peroxydicarbonate D153	23246-96-0	ridelline R14
19937-59-8	metoxuron M325	23255-93-8	hycanthone H84
20019-64-1	5,5-dimethyl-2(5 <i>H</i>)-furanone D417	23422-53-9	formetanate hydrochloride F103
20048-27-5	Bandrowski's base B2	23505-41-1	pirimiphos-ethyl P209
20354-26-1	methazole M120	23541-50-6	daunomycin D23
20535-83-5	6-methoxyguanine M139	23560-59-0	heptenophos H29
20548-54-3	calcium sulfide C46	23564-05-8	thiophanate-methyl T138
20679-58-7	1,4-bis(bromoacetoxyl)-2-butene B114	23564-06-9	thiophanate T137
20706-25-6	2-propoxyethanol acetate P317	23593-75-1	clotrimazole C365
20816-12-0	osmium tetroxide O39	23745-86-0	potassium fluoroacetate P249
20830-75-5	digoxin D339	23746-34-1	potassium bis(2-hydroxyethyl)dithiocarbamate P240
20830-81-3	daunomycin D23	23947-60-6	ethirimol E70
20831-76-9	gentiopicrin G10	23950-58-5	propyzamide P339
20859-73-8	aluminium phosphide A104	24017-47-8	triazophos T205
20917-49-1	<i>N</i> -nitrosoheptamethyleneimine N159	24151-93-7	piperophos P205
20940-37-8	2,4- <i>D</i> , diethylamine salt D7	24458-48-8	<i>N</i> -(2-methyl-2-nitropropyl)-4-nitrosoaniline M266
20941-65-5	ethyl tellurac E174	24468-13-1	2-ethylhexyl chloroformate E133
21087-64-9	metribuzin M326	24539-56-8	monopentyl phthalate M347
21112-37-8	2- <i>tert</i> -butyl-1,4-dimethoxybenzene B256	24554-26-5	<i>N</i> -[4-(5-nitro-2-furyl)-2-thiazolyl]formamide N118
21351-79-1	caesium hydroxide C17	24613-03-4	<i>N</i> -chloroaniline C157
21368-68-3	(±)-camphor C53	24634-61-5	potassium sorbate P263
21548-32-3	fosthietan F109	24691-80-3	fenfuram F10
21564-17-0	2-(thiocyanatomethylthio)benzothiazole T125	24807-55-4	3-nitro-1,2,4-triazole N182
21609-90-5	leptophos L35	24934-91-6	chlormephos C140
21725-46-2	cyanazine C480	25013-15-4	methylstyrene M306
21739-91-3	cytembena C547	25013-16-5	butylated hydroxyanisole B244
21757-82-4	plifenate P215	25057-89-0	bentazone B38
21908-53-2	mercury(II) oxide M82	25103-58-6	<i>tert</i> -dodecanethiol D587
21923-23-9	chlorthiophos C321	25154-52-3	nonylphenol (mixed isomers) N198
22071-15-4	ketoprofen K10	25154-54-5	dinitrobenzene (mixed) D473
22204-53-1	naproxen N29	25155-15-1	cymene C537
22212-55-1	benzoylprop-ethyl B84	25155-30-0	sodium dodecylbenzenesulfonate S65

25167-70-8	2,4,4-trimethylpentene T317	27193-86-8	dodecylphenol D591
25168-26-7	2,4-D, isooctyl ester D10	27253-26-5	diisotridecyl phthalate D361
25265-71-8	dipropylene glycol D555	27314-13-2	norflurazon N206
25311-71-1	isofenphos I103	27355-22-2	phthalide P174
25316-40-9	doxorubicin hydrochloride D597	27478-34-8	dinitronaphthalene D480
25319-90-8	MCPA-thioethyl M33	27774-13-6	vanadyl sulfate V16
25321-14-6	dinitrotoluene D497	28014-46-2	polyestradiol phosphate P223
25322-20-7	tetrachloroethane T48	28249-77-6	thiobencarb T117
25322-68-3	polyethylene glycol P225	28300-74-5	antimonyl potassium tartrate hemihydrate A222
25402-06-6	cinerin I C344		
25550-58-7	dinitrophenol D484	28407-37-6	C.I. Direct Blue 218 C406
25606-41-1	propamocarb hydrochloride P291	28434-86-8	4,4'-oxybis(2-chloroaniline) O54
25639-42-3	methylcyclohexanol M198	28623-46-3	nonadecanenitrile N191
25808-74-6	lead hexafluorosilicate L23	28652-72-4	methylbiphenyl M168
25954-13-6	fosamine-ammonium F107	28728-55-4	6,3-ionene I56
26002-80-2	phenothrin P84	28772-56-7	bromadiolone B152
26027-38-3	nonoxynol N196	28822-58-4	isobutylmethylxanthine I93
26049-68-3	2-hydrazino-4-(5-nitro-2-furyl)thiazole H92	29059-07-2	tetralone T82
		29091-05-2	dinitramine D466
26049-69-4	2-(2,2-dimethylhydrazino)-4-(5-nitro-2-furyl)thiazole D423	29091-21-2	prodiamine P278
		29104-30-1	benzoximate B81
26049-70-7	2-hydrazino-4-(<i>p</i> -nitrophenyl)thiazole H93	29232-93-7	pirimiphos-methyl P210
26049-71-8	2-hydrazino-4-(<i>p</i> -aminophenyl)thiazole H90	29343-52-0	4-hydroxy-2-nonenal H114
		29385-43-1	4(<i>or</i> 5)-methylbenzotriazole M164
26087-47-8	iprobefos I61	29387-86-8	butoxypropanol B230
26140-60-3	terphenyl T28	29387-92-6	<i>N,N</i> -dimethylaminoazobenzene D386
26148-68-5	A- α -C A1	29611-03-8	aflatoxicol A52
26171-83-5	1,2-butanediol B202	29929-77-9	<i>N</i> -nitroso-2,2,4-trimethyl-1,2-dihydroquinoline, polymers N176
26172-55-4	5-chloro-2-methyl-4-isothiazolinone C212		
26225-79-6	ethofumesate E72	29973-13-5	ethiofencarb E67
26249-12-7	dibromobenzene D123	30043-49-3	ethidimuron E64
26264-06-2	calcium dodecylbenzenesulfonate C32	30525-89-4	paraformaldehyde P8
26266-68-2	2-ethylhexenal E129	30560-19-1	acephate A5
26305-03-3	pepstatin A P50	30674-80-7	methacryloyloxyethyl isocyanate M110
26399-36-0	profluralin P281	30748-29-9	feprazone F29
26401-97-8	dioctyltin bis(isooctyl thioglycolate) D522	30777-18-5	benzo[<i>a</i>]fluorene B60
26419-73-8	tirpate T163	31005-02-4	7-ethoxycoumarin E75
26447-14-3	cresyl glycidyl ether C460	31217-72-8	<i>N</i> -ethyl-2-methylmaleimide E148
26471-62-5	toluene diisocyanate T175	31218-83-4	propetamphos P304
26530-20-1	octhilinone O19	31251-03-3	fluotrimazole F81
26545-73-3	dichlorohydrin D219	31512-74-0	polixetonium chloride P217
26628-22-8	sodium azide S47	31717-87-0	dodemorph acetate D593
26644-46-2	triforine T295	31879-05-7	fenoprofen F13
26675-46-7	isoflurane I105	31895-22-4	thiocyclam hydrogen oxalate T126
26761-40-0	diisodecyl phthalate D355	32809-16-8	procymidone P277
26762-92-5	<i>p</i> -menthane hydroperoxide M52	32830-97-0	1-chloro-3-pentanone C235
26780-96-1	acetanil A16	32861-85-1	chlomethoxyfen C106
26787-78-0	amoxycillin A192	33089-61-1	amitraz A158
26952-21-6	6-methyl-1-heptanol M229	33213-65-9	β -endosulfan E20
27137-85-5	dichlorophenyltrichlorosilane D243	33229-34-4	HC Blue No. 2 H8
27176-87-0	dodecylbenzenesulfonic acid D589	33629-47-9	butralin B232
27193-28-8	<i>tert</i> -octylphenol O23	33693-04-8	terbumeton T23

33719-74-3	3,5-dichloroanisole	D186	39801-14-4	photomirex	P169
33820-53-0	isopropalin	I117	40487-42-1	pendimethalin	P20
33857-26-0	dibenzo- <i>p</i> -dioxin, 2,7-dichloro-	D105	40596-69-8	methoprene	M127
33880-83-0	β -elemene	E14	41083-11-8	azocyclotin	A270
33979-15-6	clivorine	C355	41198-08-7	profenofos	P279
34014-18-1	tebuthiuron	T13	41205-09-8	hydroprene	H106
34123-59-6	isoproturon	I133	41205-21-4	fluoromide	F67
34205-21-5	dimefuron	D368	41295-28-7	methoxyphenone	M145
34256-82-1	acetochlor	A14	41394-05-2	metamitron	M95
34314-83-5	2,3-dihydro-4-methylfuran	D345	41483-43-6	bupirimate	B193
34590-94-8	dipropylene glycol methyl ether	D556	41814-78-2	tricyclazole	T272
34643-46-4	prothiofos	P341	42397-64-8	1,6-dinitropyrene	D492
34681-10-2	butocarboxim	B223	42397-65-9	1,8-dinitropyrene	D493
34681-23-7	butoxycarboxim	B225	42509-80-8	isazofos	I79
35367-38-5	diflubenzuron	D326	42576-02-3	bifenox	B108
35400-43-2	sulprofos	S159	42609-52-9	dymron	D603
35465-71-5	phenylnaphthalene	P122	42609-73-4	methyl dymron	M209
35554-44-0	imazalil	I4	42874-03-3	oxyfluorfen	O59
35575-96-3	azamethiphos	A259	42934-53-2	dibenzofuran, chlorinated	D112
35597-43-4	bilanafos	B110	43031-79-4	dichloroisopropyl ether	D221
35658-65-2	cadmium chloride monohydrate	C6	43222-48-6	difenzoquat metilsulfate	D325
35691-65-7	2-bromo-2-(bromomethyl)pentanedinitrile	B163	50375-10-5	2,3,6-trichloroanisole	T237
36335-67-8	butamifos	B198	50471-44-8	vinclozolin	V23
36356-20-4	3-chloro-4-diethylaminobenzenediazonium trichlorozincate	C190	50512-35-1	isoprothiolane	I132
36519-00-3	phosdiphen	P150	50563-36-5	dimethachlor	D371
36653-82-4	cetyl alcohol	C102	50594-66-6	acifluorfen	A30
36679-74-0	2,2,4-trimethylpentyl isobutyrate	T319	50782-69-9	VX	V41
36731-40-5	2,5(<i>or</i> 2,6)-dimethylpyrazine	D453	50864-67-0	barium polysulfides (Ba ₄ S ₇)	B23
36734-19-7	iprodione	I62	51131-85-2	9-hydroxyellipticine	H110
36756-79-3	tiocarbazil	T162	51218-45-2	metolachlor	M323
37764-25-3	dichlormid	D171	51234-28-7	benoxaprofen	B34
37893-02-0	flubenzimine	F40	51235-04-2	hexazinone	H69
37894-46-5	etacelasil	E54	51249-05-9	buminafos	B192
37924-13-3	perfluidone	P54	51308-54-4	buthiobate	B221
38178-38-0	dibenzo- <i>p</i> -dioxin, 1,6-dichloro-	D109	51338-27-3	diclofop-methyl	D259
38260-54-7	etrimfos	E186	51365-15-2	cyclopentane-1,2,3,4-tetracarboxylic acid	C523
38434-77-4	ethylnitrosocyanamide	E157	51395-10-9	copper EDTA	C436
38571-73-2	1,2,3-tris(chloromethoxy)propane	T351	51487-69-5	cloethocarb	C356
38727-55-8	diethatyl-ethyl	D282	51630-58-1	fenvalerate	F28
38777-13-8	nitrosopropoxur	N173	52315-07-8	cypermethrin	C542
39148-24-8	fosetyl-aluminium	F108	52508-35-7	dikegulac-sodium	D362
39156-41-7	2,4-diaminoanisole sulfate	D74	52645-53-1	permethrin	P56
39196-18-4	thiofanox	T131	52740-16-6	calcium arsenite	C23
39202-40-9	iminoctadine	I10	52756-25-9	flamprop-methyl	F340
39227-53-7	dibenzo- <i>p</i> -dioxin, 1-chloro-	D107	52888-80-9	prosulfofocarb	P340
39227-54-8	dibenzo- <i>p</i> -dioxin, 2-chloro-	D108	52918-63-5	deltamethrin	D46
39300-45-3	dinocap	D505	53111-28-7	barium polysulfides (Ba ₂ S ₃)	B22
39603-48-0	1,1'-methylenebis(thiosemicarbazide)	M215	53469-21-9	Aroclor 1242	A236
39765-80-5	<i>trans</i> -nonachlor	N190	53558-25-1	pyrinuron	P362
			53609-64-6	<i>N</i> -nitrosodiisopropanolamine	N151
			53780-34-0	mefluidide	M43

53924-05-3	7-chloroindole C205	61213-25-0	flurochloridone F87
54135-80-7	2,3,4-trichloroanisole T235	61702-44-1	2-chloro- <i>p</i> -phenylenediamine sulfate C243
54135-81-8	2,3,5-trichloroanisole T236	61788-33-8	polychlorinated terphenyls P220
54150-69-5	2,4-dimethoxyaniline hydrochloride D378	61789-65-9	aluminium resinate A106
54350-48-0	etretinate E184	61790-53-2	diatomaceous earth D97
54453-03-1	EDTA copper complex E5	61791-55-7	<i>N</i> -tallow-1,3-propanediamine T4
54749-90-5	chlorozotocin C307	62450-06-0	Trp-P-1 T364
54788-38-4	3-chloro-4-methylanisole C207	62450-07-1	Trp-P-2 T365
55069-01-7	Eulan WA new E188	62610-77-9	methacrifos M102
55179-31-2	bitertanol B137	62850-32-2	fenothiocarb F15
55219-65-3	triadimenol T197	62924-70-3	flumetralin F45
55283-68-6	ethalfuralin E56	63148-62-9	silicone oil S32
55285-14-8	carbosulfan C83	63284-71-9	nuarimol N209
55290-64-7	dimethipin D374	63333-35-7	bromethalin B153
55335-06-3	triclopyr T271	63412-06-6	<i>N</i> -methyl- <i>N</i> -nitrosobenzamide M267
55512-33-9	pyridate P356	63449-39-8	chlorinated paraffins C132
55557-00-1	dinitrosohomopiperazine D494	63449-41-2	alkyl(C ₁₄ -C ₁₆)dimethylbenzylammonium chloride A66
55814-41-0	mepronil M58	63642-17-1	<i>N</i> -(<i>N</i> -methyl- <i>N</i> -nitrosocarbamoyl)- <i>L</i> -ornithine M268
55861-78-4	isouron I139	63782-90-1	flampropr-M-isopropyl F35
55965-85-0	5-chloro-2-methyl-4-isothiazolinone calcium chloride complex C213	63937-14-4	mercury gluconate M74
56073-07-5	difenacoum D323	64091-91-4	NNK N189
56073-10-0	brodifacoum B150	64249-01-0	anilofos A212
56323-17-2	tributyltin fumarate T216	64257-84-7	fenpropathrin F18
56425-91-3	flurprimidol F89	64902-72-3	chlorsulfuron C315
56654-52-5	1,3-dibutyl-1-nitrosourea D149	65277-42-1	ketoconazole K9
56717-11-4	piproctanyl bromide P206	65907-30-4	furathiocarb F125
56894-91-8	bis-1,4-(chloromethoxy)- <i>p</i> -xylene B122	65996-93-2	coal tar volatiles (benzene-soluble) C367
57208-09-0	cobalt naphthoate C375	65997-15-1	cement, Portland C99
57369-32-1	pyroquilon P365	66003-55-2	alloydim-sodium A71
57646-30-7	furalaxyl F119	66063-05-6	pencycuron P19
57653-85-7	1,2,3,6,7,8-hexachlorodibenzo- <i>p</i> -dioxin H36	66215-27-8	cyromazine C545
57835-92-4	4-nitropyrene N143	66230-04-4	esfenvalerate E49
57837-19-1	metalaxyl M93	66246-88-6	penconazole P18
57917-55-2	Beetroot Red B25	66332-96-5	flutolanil F92
57966-95-7	cymoxanil C541	66441-23-4	fenoxaprop-ethyl F16
58769-20-3	kadethrin K1	66733-21-9	erionite E45
58810-48-3	ofurace O26	66841-25-6	tralomethrin T194
59080-40-9	2,2',4,4',5,5'-hexabromobiphenyl H31	67129-08-2	metazachlor M98
59333-67-4	fluoxetine hydrochloride F82	67306-00-7	fenpropidin F19
59536-65-1	polybrominated biphenyls P219	67375-30-8	α -cypermethrin C543
59643-77-5	calcium <i>o</i> -iodoxybenzoate C35	67485-29-4	hydramethylnon H86
59669-26-0	thiodicarb T128	67564-91-4	fenpropimorph F20
59756-60-4	fluridone F86	67730-10-3	Glu-P-2 G20
59865-13-3	cyclosporin A C531	67730-11-4	Glu-P-1 G19
60168-88-9	fenarimol F4	67747-09-5	prochloraz P275
60207-31-0	azaconazole A256	67774-32-7	polybrominated biphenyls P219
60207-90-1	propiconazole P306	68085-85-8	cyhalothrin C534
60207-93-4	etaconazole E55	68107-26-6	<i>N</i> -nitroso- <i>N</i> -methylundecylamine N162
60238-56-4	chlorthiophos C321	68228-18-2	proglinazine-ethyl P283
60568-05-0	furmecyclox F130	68359-37-5	cyfluthrin C533

68476-85-7	LPG	L59	
68603-42-9	cocamide DEA	C381	
68956-82-1	cobalt resinate	C377	
69327-76-0	buprofezin	B194	
69377-81-7	fluroxypyr	F88	
69581-33-5	cyprofuram	C544	
69655-05-6	didanosine	D273	
69806-50-4	fluazifop-butyl	F38	
70124-77-5	flucythrinate	F43	
70657-70-4	2-methoxypropanol acetate	M149	
71626-11-4	benalaxyl	B26	
72178-02-0	fomesafen	F98	
73250-68-7	mefenacet	M41	
73909-16-7	6-chloro-3-methylanisole	C209	
74051-80-2	sethoxydim	S25	
74070-46-5	aclonifen	A32	
74115-24-5	clofentezine	C357	
74222-97-2	sulfometuron-methyl	S145	
74223-64-6	metsulfuron-methyl	M328	
74712-19-9	bromobutide	B166	
74782-23-3	oxabetrinil	O42	
74920-78-8	N-ethyl-N-formylhydrazine	E124	
75485-12-0	1-azetidinecarbonyl chloride	A262	
76543-88-9	interferon alfa	I39	
76674-21-0	flutriafol	F93	
76714-88-0	diniconazole	D464	
76738-62-0	paclobutrazol	P1	
77094-11-2	MeIQ	M45	
77182-82-2	glufosinate-ammonium	G18	
77458-01-6	pyraclofos	P347	
77500-04-0	MeIQx	M46	
77501-90-7	fluoroglycofen-ethyl	F66	
77732-09-3	oxadixyl	O45	
78587-05-0	hexythiazox	H80	
79127-80-3	fenoxycarb	F17	
79241-46-6	fluazifop-P-butyl	F39	
79538-32-2	tefluthrin	T15	
79983-71-4	hexaconazole	H43	
81334-34-1	imazapyr	I6	
81335-77-5	imazethapyr	I7	
81405-85-8	imazamethabenz-methyl	I5	
81412-43-3	tridemorph	T273	
81777-89-1	clomazone	C359	
82560-54-1	benfuracarb	B30	
82657-04-3	bifenthrin	B109	
83130-01-2	alanycarb	A61	
83164-33-4	diflufenican	D327	
83463-62-1	bromochloroacetonitrile	B167	
84332-86-5	chlozolate	C322	
85509-19-9	flusilazol	F90	
87130-20-9	diethofencarb	D283	
87237-48-7	haloxyfop-ethoxyethyl	H5	
88283-41-4	pyrifenoxy	P360	
88485-37-4	fluxofenim	F95	
88671-89-0	myclobutanil	M360	
89269-64-7	ferimzone	F31	
90035-08-8	flocoumafen	F37	
95465-99-9	cadusafos	C15	
97780-06-8	ethametsulfuron-methyl	E57	
99387-89-0	triflumizole	T289	
100760-10-9	quizalofop-ethyl	Q13	
102851-06-9	τ -fluvalinate	F94	
104078-12-8	dinocton	D506	
105650-23-5	PhIP	P144	
106917-52-6	flusulfamide	F91	
107534-96-3	tebuconazole	T11	
108171-26-2	chlorinated paraffins (C ₁₂ , 60% Cl)	C133	
108171-27-3	chlorinated paraffins (C ₂₃ , 43% Cl)	C134	
111479-05-1	propaquizafop	P299	
111812-58-9	fenpyroximate	F21	
112281-77-3	tetraconazole	T61	
112410-23-8	tebufenozide	T12	
115044-19-4	guazatine acetates	G52	
120068-37-3	fipronil	F33	
120928-09-8	fenazaquin	F6	
136677-10-6	dibenzofuran, polychlorinated	D113	
138261-41-3	imidacloprid	I8	

Index of Molecular Formulae

Ag	silver S33	$B_4H_{20}Na_2O_{17}$	borax B141
AgCN	silver cyanide S35	$B_4Na_2O_7$	sodium tetraborate S96
AgNO ₃	silver nitrate S36	B_5H_9	pentaborane(9) P23
Ag ₃ AsO ₃	silver arsenite S34	$B_{10}H_{14}$	decaborane D37
Al	aluminium A96	Ba	barium B5
AlBr ₃	aluminium bromide A97	BaBr ₂	barium bromide B8
AlCl ₃	aluminium chloride A99	BaBr ₂ O ₆	barium bromate B7
AlF ₆ Na ₃	cryolite C472	BaCO ₃	barium carbonate B9
AlH ₃	aluminium hydride A100	BaC ₂ N ₂	barium cyanide B12
AlH ₄ Li	lithium aluminium hydride L53	BaCl ₂	barium chloride B11
AlKO ₈ S ₂	aluminium potassium sulfate A105	BaCl ₂ O ₆	barium chlorate B10
AlN ₃ O ₉ H ₁₈ O ₉	aluminium nitrate nonahydrate A102	BaCl ₂ O ₈	barium perchlorate B15
AlP	aluminium phosphide A104	BaMn ₂ O ₈	barium permanganate B16
Al ₂ H ₄ O ₉ Si ₂	kaolin K2	BaN ₂ O ₆	barium nitrate B13
Al ₂ O ₃	aluminium oxide A103	BaO	barium oxide B14
Al ₂ O ₁₂ S ₃	aluminium sulfate A107	BaO ₂	barium peroxide B17
Al ₄ C ₃	aluminium carbide A98	BaO ₄ S	barium sulfate B24
As	arsenic A240	BaS ₂	barium polysulfides (BaS ₂) B18
AsCl ₃	arsenic trichloride A243	BaS ₃	barium polysulfides (BaS ₃) B19
AsHO ₄ Pb	lead arsenate L13	BaS ₄	barium polysulfides (BaS ₄) B20
AsH ₂ KO ₄	potassium arsenate P238	BaS ₅	barium polysulfides (BaS ₅) B21
AsH ₃	arsine A246	Ba ₂ S ₃	barium polysulfides (Ba ₂ S ₃) B22
AsH ₃ O ₄	arsenic acid A241	Ba ₄ S ₇	barium polysulfides (Ba ₄ S ₇) B23
AsH ₃ O ₄ Mgx	magnesium arsenate M2	Be	beryllium B102
AsH ₉ N ₂ O ₄	ammonium arsenate A163	BeCl ₂	beryllium chloride B103
AsNaO ₂	sodium arsenite S45	BeF ₂	beryllium fluoride B104
As ₂ Ca ₃ O ₆	calcium arsenite C23	BeN ₂ O ₆	beryllium nitrate B105
As ₂ Ca ₃ O ₈	calcium arsenate C22	BeO ₄ S	beryllium sulfate B106
As ₂ HKO ₄	potassium arsenite P239	Bi ₂ Te ₃	bismuth telluride B132
As ₂ O ₃	arsenic trioxide A244	BrCl	bromine chloride B155
As ₂ O ₄ Pb	lead arsenite L14	BrF ₃	bromine trifluoride B157
As ₂ S ₂	arsenic disulfide A242	BrF ₅	bromine pentafluoride B156
As ₂ S ₃	arsenic trisulfide A245	BrKO ₃	potassium bromate P241
At	astatine A250	BrNaO ₃	sodium bromate S51
Au	gold G42	Br ₂	bromine B154
AuCl ₃	gold trichloride G43	Br ₂ Co	cobalt(II) bromide C370
BBr ₃	boron tribromide B145	Br ₂ Zn	zinc bromide Z4
BCl ₃	boron trichloride B146	Br ₃ P	phosphorus tribromide P165
BF ₃	boron trifluoride B147	Br ₄ C	carbon tetrabromide C77
BF ₄ H	fluoboric acid F46	C	carbon black C73
BH ₄ Na	sodium borohydride S50	C	graphite G45
B ₂ F ₆ Pb	lead fluoborate L21	CBrClF ₂	bromochlorodifluoromethane B168
B ₂ H ₆	diborane D121	CBrF ₃	bromotrifluoromethane B188
B ₂ O ₃	boron oxide B144	CBrN	cyanogen bromide C483
		CBr ₂ Cl ₂	dibromodichloromethane D130

CBr_2F_2	dibromodifluoromethane D131	$\text{CH}_4\text{Cl}_2\text{Si}$	dichloromethylsilane D225
CBr_3NO_2	tribromonitromethane T206	$\text{CH}_4\text{N}_2\text{O}$	urea U12
CCaN_2	calcium cyanamide C29	$\text{CH}_4\text{N}_2\text{S}$	thiourea T146
CCaO_3	calcium carbonate C25	$\text{CH}_4\text{N}_2\text{S}$	ammonium thiocyanate A190
CClF_3	chlorotrifluoromethane C302	$\text{CH}_4\text{N}_2\text{Se}$	selenourea S21
CCIN	cyanogen chloride C484	$\text{CH}_4\text{N}_4\text{O}_2$	nitroguanidine N122
CCl_2F_2	dichlorodifluoromethane D204	CH_4O	methanol M116
CCl_2O	phosgene P152	$\text{CH}_4\text{O}_3\text{S}$	methanesulfonic acid M113
CCl_2S	thiophosgene T140	CH_4S	methanethiol M115
CCl_3F	fluorotrichloromethane F78	CH_5N	methylamine M154
CCl_3NO_2	chloropicrin C259	CH_5NO_3	ammonium bicarbonate A165
CCl_4	carbon tetrachloride C78	$\text{CH}_5\text{N}_3\text{S}$	thiosemicarbazide T144
CCl_4S	trichloromethanesulphenyl chloride T252	CH_6ClN_3	guanidine hydrochloride G48
		$\text{CH}_6\text{ClN}_3\text{O}$	semicarbazide hydrochloride S22
CCuN	copper(i) cyanide C435	CH_6N_2	methylhydrazine M234
CF_2O	carbonyl fluoride C80	$\text{CH}_6\text{N}_2\text{O}_2$	ammonium carbamate A167
CF_4	carbon tetrafluoride C79	$\text{CH}_6\text{N}_4\text{O}$	carbohydrazide C69
CHBrCl_2	bromodichloromethane B173	$\text{CH}_6\text{N}_4\text{O}_3$	guanidine nitrate G49
CHBr_2Cl	dibromochloromethane D126	$\text{CH}_6\text{N}_4\text{S}$	thiocarbazine T124
CHBr_3	bromoform B177	$\text{CH}_8\text{N}_2\text{O}_3$	ammonium carbonate A168
CHClF_2	chlorodifluoromethane C192	$\text{CH}_8\text{N}_2\text{O}_4\text{S}$	methylhydrazine sulfate M235
CHCl_2F	dichlorofluoromethane D216	ClN	cyanogen iodide C485
CHCl_2I	dichloriodomethane D220	CKN	potassium cyanide P245
CHCl_3	chloroform C201	CN	cyanide C481
CHF_3	trifluoromethane T292	CNNa	sodium cyanide S58
CHI_3	iodoform I51	CN_4O_8	tetranitromethane T95
CHN	hydrogen cyanide H100	CN_2O_3	sodium carbonate S52
CH_2BrCl	bromochloromethane B171	CO	carbon monoxide C76
CH_2Br_2	dibromomethane D133	COS	carbonyl sulfide C81
CH_2ClF	chlorofluoromethane C200	CO_2	carbon dioxide C74
CH_2Cl_2	dichloromethane D222	CO_3Ti_2	thallium(i) carbonate T102
$\text{CH}_2\text{Cl}_4\text{Si}$	trichloro(chloromethyl)silane T246	CO_3Zn	zinc carbonate Z5
		CS_2	carbon disulfide C75
CH_2N_2	diazomethane D100	CSi	silicon carbide S31
CH_2N_2	cyanamide C479	CW	tungsten carbide T372
$(\text{CH}_2\text{O})_n$	paraformaldehyde P8	C_2AgKN_2	potassium silver cyanide P262
CH_2O	formaldehyde F100	C_2CaN_2	calcium cyanide C30
CH_2O_2	formic acid F104	C_2ClF_3	chlorotrifluoroethylene C301
$\text{CH}_3\text{AsNa}_2\text{O}_3$	DSMA D601	C_2ClF_5	chloropentafluoroethane C234
CH_3Br	bromomethane B178	C_2Cl_2	dichloroacetylene D177
CH_3Cl	chloromethane C206	$\text{C}_2\text{Cl}_2\text{F}_4$	1,2-dichlorotetrafluoroethane D252
$\text{CH}_3\text{Cl}_2\text{OP}$	methylphosphonic dichloride M287	$\text{C}_2\text{Cl}_3\text{F}_3$	1,1,2-trichlorotrifluoroethane T269
$\text{CH}_3\text{Cl}_3\text{Si}$	methyltrichlorosilane M314	$\text{C}_2\text{Cl}_3\text{N}$	trichloroacetonitrile T229
$\text{CH}_3\text{FO}_2\text{S}$	methanesulfonyl fluoride M114	$\text{C}_2\text{Cl}_3\text{NaO}_2$	sodium trichloroacetate S97
$\text{CH}_3\text{FO}_3\text{S}$	methyl fluorosulfonate M224	C_2Cl_4	tetrachloroethylene T51
CH_3Hg	methylmercury M249	$\text{C}_2\text{Cl}_4\text{F}_2$	1,2-difluorotetrachloroethane D334
CH_3I	iodomethane I52		1,1-difluorotetrachloroethane D333
CH_3NO	formamide F101		trichloroacetyl chloride T230
CH_3NO_2	nitromethane N127		hexachloroethane H38
CH_4	methane M112		
$\text{CH}_4\text{AsO}_3\text{Na}$	MSMA M355		

C_2CuO_4	copper oxalate C439	$C_2H_3ClO_2$	methyl chloroformate M188
C_2F_4	tetrafluoroethylene T70	$C_2H_3Cl_2NO_2$	1,1-dichloro-1-nitroethane D232
$(C_2F_4)_n$	polytetrafluoroethylene P232	$C_2H_3Cl_3$	1,1,1-trichloroethane T247
C_2F_6	hexafluoroethane H46	$C_2H_3Cl_3$	1,1,2-trichloroethane T248
$C_2HBrClF_3$	halothane H4	$C_2H_3Cl_3O_2$	chloral hydrate C108
$C_2HBrClIN$	bromochloroacetonitrile B167	$C_2H_3Cl_3Si$	vinyltrichlorosilane V39
C_2HBr_2N	dibromoacetonitrile D122	C_2H_3F	vinyl fluoride V33
C_2HCl_2N	dichloroacetonitrile D175	$C_2H_3FO_2$	fluoroacetic acid F55
C_2HCl_3	trichloroethylene T249	C_2H_3IO	acetyl iodide A27
C_2HCl_3O	dichloroacetyl chloride D176	$C_2H_3IO_2$	iodoacetic acid I42
C_2HCl_3O	chloral C107	C_2H_3N	acetonitrile A20
$C_2HCl_3O_2$	trichloroacetic acid T226	C_2H_3NO	methyl isocyanate M243
C_2HCl_5	pentachloroethane P28	C_2H_3NO	glycolonitrile G37
$C_2HF_3O_2$	trifluoroacetic acid T290	C_2H_3NS	methyl isothiocyanate M245
C_2H_2	acetylene A26	C_2H_3NS	methyl thiocyanate M310
$C_2H_2AsCl_3$	Lewisite L41	$C_2H_3N_3$	1,2,4-triazole T204
C_2H_2BrN	bromoacetonitrile B159	$C_2H_3NaO_2$	sodium acetate S40
$C_2H_2Br_4$	1,1,2,2-tetrabromoethane T40	$C_2H_3O_2Tl$	thallium(I) acetate T101
C_2H_2ClFO	fluoroacetyl chloride F56	C_2H_4	ethylene E113
$C_2H_2ClF_3$	2-chloro-1,1,1-trifluoroethane C300	$(-C_2H_4-)_n$	polyethylene P224
C_2H_2ClIN	chloroacetonitrile C147	C_2H_4BrCl	1-bromo-2-chloroethane B170
$C_2H_2ClINaO_2$	sodium chloroacetate S55	$C_2H_4Br_2$	1,2-dibromoethane D132
$C_2H_2Cl_2$	1,1-dichloroethylene D212	C_2H_4ClNO	2-chloroacetamide C144
$C_2H_2Cl_2$	<i>cis</i> -1,2-dichloroethylene D213	$C_2H_4ClNO_2$	1-chloro-1-nitroethane C226
$C_2H_2Cl_2$	<i>trans</i> -1,2-dichloroethylene D214	$C_2H_4Cl_2$	1,1-dichloroethane D210
$C_2H_2Cl_2F_2$	1,2-dichloro-1,1-difluoroethane D203	$C_2H_4Cl_2$	1,2-dichloroethane D211
$C_2H_2Cl_2O$	chloroacetyl chloride C151	$C_2H_4Cl_2O$	bis(chloromethyl) ether B123
$C_2H_2Cl_2O_2$	dichloroacetic acid D172	C_2H_4FNO	fluoroacetamide F53
$C_2H_2Cl_4$	1,1,2,2-tetrachloroethane T50	$C_2H_4F_2$	1,1-difluoroethane D330
$C_2H_2Cl_4$	tetrachloroethane T48	$C_2H_4F_2$	1,2-difluoroethane D331
$C_2H_2Cl_4$	1,1,1,2-tetrachloroethane T49	$C_2H_4NNaS_2$	metam-sodium M96
$C_2H_2CoO_4$	cobalt(III) formate C373	$C_2H_4N_2O_6$	ethylene dinitrate E115
$C_2H_2FKO_2$	potassium fluoroacetate P249	$C_2H_4N_4$	amitrole A160
$C_2H_2FNaO_2$	sodium fluoroacetate S67	$C_2H_4N_4O_2$	azodicarbonamide A271
$C_2H_2F_2$	1,1-difluoroethylene D332	$C_2H_4Na_2O_7P_2$	disodium etidronate D562
$C_2H_2N_4O_2$	3-nitro-1,2,4-triazole N182	C_2H_4O	ethylene oxide E120
C_2H_2O	ketene K8	C_2H_4O	acetaldehyde A7
$C_2H_2O_2$	glyoxal G39	C_2H_4O	vinyl alcohol V27
$C_2H_2O_4$	oxalic acid O46	$(C_2H_4O)_n$	polyvinyl alcohol P234
$C_2H_2O_4Cd$	cadmium formate C9	$(-C_2H_4O-)_nH_{20}$	polyethylene glycol P225
$C_2H_3As_3Cu_2O_8$	copper acetoarsenite C431	C_2H_4OS	thioacetic acid T116
C_2H_3Br	vinyl bromide V28	$C_2H_4O_2$	methyl formate M226
C_2H_3BrO	acetyl bromide A24	$C_2H_4O_2$	acetic acid A12
$C_2H_3BrO_2$	bromoacetic acid B158	$C_2H_4O_2S$	mercaptoacetic acid M59
C_2H_3Cl	vinyl chloride V30	$C_2H_4O_3$	peracetic acid P51
$(C_2H_3Cl)_n$	polyvinyl chloride P235	C_2H_4S	ethylene sulfide E121
$C_2H_3ClF_2$	1-chloro-1,1-difluoroethane C191	C_2H_5Br	bromoethane B175
C_2H_3ClO	acetyl chloride A25	C_2H_5Cl	chloroethane C196
C_2H_3ClO	chloroacetaldehyde C143	C_2H_5ClHg	ethylmercury(II) chloride E143
$C_2H_3ClO_2$	chloroacetic acid C145	C_2H_5ClO	chloromethyl methyl ether C214
		C_2H_5ClO	2-chloroethanol C197
		$C_2H_5ClO_4$	ethyl perchlorate E159

$C_2H_5Cl_3Si$	ethyltrichlorosilane E180	$C_2H_7HgO_4P$	ethylmercury(II) phosphate E144
C_2H_5F	fluoroethane F64	C_2H_7N	ethylamine E90
C_2H_5FO	2-fluoroethanol F65	C_2H_7N	dimethylamine D384
C_2H_5I	iodoethane I49	C_2H_7NO	ethanolamine E62
C_2H_5N	aziridine A266	$C_2H_7NO_2$	ammonium acetate A162
C_2H_5NO	<i>N</i> -methylformamide M225	$C_2H_7O_3P$	dimethyl phosphite D449
C_2H_5NO	acetamide A10	$C_2H_8NO_2PS$	methamidophos M111
C_2H_5NO	acetaldoxime A9	$C_2H_8N_2$	1,1-dimethylhydrazine D420
$C_2H_5NO_2$	nitroethane N111	$C_2H_8N_2$	1,2-dimethylhydrazine D421
$C_2H_5NO_2$	methyl carbamate M184	$C_2H_8N_2$	ethylenediamine E114
$C_2H_5NO_2$	ethyl nitrite E156	$C_2H_8N_2O$	2-hydrazinoethanol H91
$C_2H_5NO_2$	glycine G36	$C_2H_8N_2O_4$	diammonium oxalate D94
$C_2H_5NO_4$	ammonium oxalate A179	$C_2H_8O_7P_2$	etidronic acid E183
C_2H_5NS	thioacetamide T115	$C_2H_{10}N_2Cl_2$	1,2-dimethylhydrazine dihydrochloride D422
$C_2H_5N_3O_2$	1-nitroso-1-methylurea N163	$C_2H_8N_2$	mercury(II) cyanide M72
$C_2H_5N_3S_2$	2,4-dithiobiuret D574	$C_2H_8N_2O_2$	mercury fulminate M73
$C_2H_5N_5O_3$	1-methyl-3-nitro-1-nitrosoguanidine M265	$C_2H_8N_2S_2$	mercury(II) thiocyanate M87
C_2H_6	ethane E58	$C_2H_8N_2O$	mercury oxycyanide M83
$C_2H_6AsNaO_2$	sodium dimethylarsinate S63	C_2N_2	cyanogen C482
$C_2H_6BF_3O$	boron trifluoride dimethyl etherate B149	C_2N_2Pb	lead cyanide L17
$C_2H_6ClNO_2S$	dimethylaminosulfonyl chloride D393	$C_2N_2S_2Pb$	lead thiocyanate L33
$C_2H_6ClO_2PS$	dimethyl chlorothiophosphate D407	C_2N_2Zn	zinc cyanide Z8
$C_2H_6ClO_3P$	ethephon E63	$C_3Cl_3N_3$	cyanuric chloride C492
$C_2H_6Cl_2Si$	dichlorodimethylsilane D206	$C_3Cl_3N_3O_3$	trichloroisocyanuric acid T250
C_2H_6Hg	dimethylmercury D427	C_3Cl_6	hexachloropropene H42
$C_2H_6N_2O$	<i>N</i> -methyl- <i>N</i> -formylhydrazine M227	C_3Cl_6O	hexachloroacetone H32
$C_2H_6N_2O$	dimethylnitrosamine D444	$C_3F_3N_3$	cyanuric fluoride C493
$C_2H_6N_2O$	methylurea M315	C_3F_6	hexafluoropropene H48
$C_2H_6N_2O_2$	methylazoxymethanol M159	C_3F_6O	hexafluoroacetone H45
$C_2H_6N_2O_2$	dimethylnitramine D443	C_3F_8	octafluoropropane O7
$C_2H_6N_4S_2$	2,5-dithiobiurea D573	$C_3HCl_2N_3O_3$	dichlorocyanuric acid D202
C_2H_6O	dimethyl ether D413	C_3HCl_5O	pentachloroacetone P25
C_2H_6O	ethanol E61	$C_3HF_4NaO_2$	flupropionate-sodium F83
C_2H_6OS	dimethyl sulfoxide D458	$C_3H_2Br_2N_2O$	2,2-dibromo-3-nitrilopropionamide D135
C_2H_6OS	2-mercaptoethanol M62	$C_3H_2ClF_5O$	enflurane E27
$(C_2H_6OSi)_x$	polydimethylsiloxane P222	$C_3H_2ClF_5O$	isoflurane I105
$C_2H_6O_2$	ethylene glycol E116	C_3H_2ClN	2-chloroacrylonitrile C152
$C_2H_6O_2S$	dimethyl sulfone D457	$C_3H_2Cl_4$	1,1,2,3-tetrachloropropene T59
$C_2H_6O_3S$	methyl methanesulfonate M253	$C_3H_2Cl_4O$	1,1,3,3-tetrachloroacetone T43
$C_2H_6O_4S$	ethylsulfuric acid E173	$C_3H_2F_6O$	1,1,1,3,3,3-hexafluoro-2-propanol H47
$C_2H_6O_4S$	dimethyl sulfate D455	$C_3H_2N_2$	malononitrile M18
C_2H_6S	dimethyl sulfide D456	$C_3H_2O_4Ti_2$	thallium(I) malonate T105
C_2H_6S	ethanethiol E60	C_3H_3Cl	3-chloropropyne C278
$C_2H_6S_2$	ethanedithiol E59	C_3H_3ClO	acryloyl chloride A44
$C_2H_6S_2$	dimethyl disulfide D412	$C_3H_3Cl_2NaO_2$	dalapon-sodium D20
C_2H_6Zn	dimethylzinc D461	$C_3H_3Cl_3$	3,3,3-trichloro-1-propene T266
$C_2H_7AsO_2$	cacodylic acid C1	$C_3H_3Cl_3$	1,2,3-trichloro-1-propene T265
		$C_3H_3Cl_3N_6$	trichloromelamine T251
		$C_3H_3Cl_3O$	1,1,1-trichloroacetone T227

$C_3H_3Cl_3O$	1,1,3-trichloroacetone T228	$C_3H_5Cl_3$	1,1,2-trichloropropane T263
$C_3H_3Cl_5$	1,1,2,3,3-pentachloropropane P32	$C_3H_5Cl_3Si$	allyltrichlorosilane A94
$C_3H_3Cl_5$	1,1,2,2,3-pentachloropropane P31	C_3H_5FO	epifluorohydrin E34
C_3H_3N	acrylonitrile A43	C_3H_5I	allyl iodide A85
C_3H_3NS	thiazole T114	C_3H_5N	propionitrile P312
$C_3H_3N_3O_2$	4-nitroimidazole N125	C_3H_5NO	acrylamide A41
$C_3H_3N_3O_2$	2-nitroimidazole N124	C_3H_5NO	ethyl isocyanate E140
$C_3H_3N_3O_2S$	2-amino-5-nitrothiazole A141	C_3H_5NO	lactonitrile L2
$C_3H_3N_3O_3$	cyanuric acid C491	$C_3H_5NO_4$	3-nitropropionic acid N140
C_3H_4	propyne P338	C_3H_5NS	ethyl thiocyanate E175
$C_3H_4Br_2O$	acrolein dibromide A38	$C_3H_5N_3O$	ethylnitrosocyanamide E157
C_3H_4ClN	2-chloropropionitrile C273	$C_3H_5N_3O_9$	glycerol trinitrate G26
C_3H_4ClN	3-chloropropionitrile C274	$C_3H_5O_2Cl$	ethyl chloroformate E107
$C_3H_4Cl_2$	1,1-dichloropropene D248	C_3H_6	cyclopropane C530
$C_3H_4Cl_2$	2,3-dichloropropene D251	C_3H_6	propene P303
$C_3H_4Cl_2$	1,3-dichloropropene D250	C_3H_6BrCl	1-bromo-3-chloropropane B172
$C_3H_4Cl_2$	1,2-dichloropropene D249	$C_3H_6BrNO_4$	bronopol B190
$C_3H_4Cl_2F_2O$	methoxyfluorane M138	$C_3H_6Br_2O$	2,3-dibromopropanol D137
$C_3H_4Cl_2O$	3-chloropropionyl chloride C275	C_3H_6ClNO	dimethylcarbamyl chloride D406
$C_3H_4Cl_2O$	1,3-dichloroacetone D174	$C_3H_6ClNO_2$	1-chloro-1-nitropropane C231
$C_3H_4Cl_2O$	1,1-dichloroacetone D173	$C_3H_6ClNO_2$	2-chloro- <i>N</i> - (hydroxymethyl)acetamide C204
$C_3H_4Cl_2O_2$	2-chloroethyl chloroformate C198	$C_3H_6Cl_2$	1,3-dichloropropane D246
$C_3H_4Cl_2O_2$	methyl dichloroacetate M205	$C_3H_6Cl_2$	1,1-dichloropropane D244
$C_3H_4Cl_2O_2$	dalapon D19	$C_3H_6Cl_2$	1,2-dichloropropane D245
$C_3H_4Cl_4$	1,2,2,3-tetrachloropropane T58	$C_3H_6Cl_2O$	1,3-dichloro-2-propanol D247
$C_3H_4Cl_4$	1,1,1,3-tetrachloropropane T57	$C_3H_6Cl_2O$	dichlorohydrin D219
$C_3H_4N_2$	imidazole I9	$C_3H_6HgN_4$	methylmercury(II) dicyandiamide M251
$C_3H_4N_2$	pyrazole P349	$C_3H_6HgO_2$	methylmercury(II) acetate M250
C_3H_4O	acrolein A35	$C_3H_6KNS_2$	potassium dimethyldithio- carbamate P247
C_3H_4O	propargyl alcohol P301	$C_3H_6NNaS_2$	sodium dimethyldithiocarbamate S64
$C_3H_4O_2$	β -propiolactone P308	$C_3H_6N_2O$	<i>N</i> -nitroso- <i>N</i> -methylvinylamine N165
$C_3H_4O_2$	acrylic acid A42	$C_3H_6N_2OS$	1-acetyl-2-thiourea A29
$C_3H_4O_2$	malonaldehyde M16	$C_3H_6N_2O_3$	<i>N</i> -nitrososarcosine N175
$C_3H_4O_2$	glycidaldehyde G27	$C_3H_6N_2O_6$	propylene glycol dinitrate P329
$C_3H_4O_3$	pyruvic acid P368	$C_3H_6N_2S$	ethylenethiourea E122
$C_3H_4O_4$	malonic acid M17	$C_3H_6N_6$	melamine M47
C_3H_5Br	allyl bromide A76	$C_3H_6N_6O_6$	RDX R2
C_3H_5BrO	epibromohydrin E32	C_3H_6O	acetone A17
$C_3H_5BrO_2$	methyl bromoacetate M171	C_3H_6O	methyl vinyl ether M317
$C_3H_5Br_2Cl$	1,2-dibromo-3-chloropropane D128	C_3H_6O	propionaldehyde P309
C_3H_5Cl	2-chloropropene C271	C_3H_6O	allyl alcohol A73
C_3H_5Cl	allyl chloride A78	C_3H_6O	trimethylene oxide T309
C_3H_5Cl	(<i>E</i>)-1-chloropropene C269	C_3H_6O	propylene oxide P330
C_3H_5ClO	(<i>Z</i>)-1-chloropropene C270	$C_3H_6O_2$	methyl acetate M151
C_3H_5ClO	chloroacetone C146	$C_3H_6O_2$	propionic acid P310
C_3H_5ClO	propionyl chloride P313	$C_3H_6O_2$	ethyl formate E123
$C_3H_5ClO_2$	epichlorohydrin E33	$C_3H_6O_2$	glycidol G28
$C_3H_5ClO_2$	2-chloropropionic acid C272		
$C_3H_5ClO_2$	methyl chloroacetate M186		
$C_3H_5Cl_3$	1,1,1-trichloropropane T262		
$C_3H_5Cl_3$	1,2,3-trichloropropane T264		

$C_3H_6O_2$	1,3-dioxolane D532	C_3H_9NO	1-amino-2-propanol A148
$C_3H_6O_2S$	methyl mercaptoacetate M248	$C_3H_9O_3P$	dimethyl methylphosphonate D430
$C_3H_6O_2S$	thiolactic acid T132		
$C_3H_6O_3$	lactic acid L1	$C_3H_9O_3P$	trimethyl phosphite T325
$C_3H_6O_3$	glyceraldehyde G23	$C_3H_9O_4P$	trimethyl phosphate T324
$C_3H_6O_3$	D-glyceraldehyde G24	$C_3H_{10}N_2$	1,2-diaminopropane D83
$C_3H_6O_3$	1,3,5-trioxane T333	$C_3H_{10}N_2$	1,3-diaminopropane D84
$C_3H_6O_3$	methoxyacetic acid M130	$C_3H_{10}N_6S_2$	1,1'-methylenebis-(thiosemicarbazide) M215
$C_3H_6O_3S$	1,3-propane sultone P293		fosamine-ammonium F107
C_3H_7Br	2-bromopropane B186	$C_3H_{11}N_2O_4P$	hydrotalcite H108
C_3H_7Br	1-bromopropane B185	$C_3H_{24}Al_2Mg_6O_{23}$	hexachlorobutadiene H34
C_3H_7Cl	1-chloropropane C263	C_4Cl_6	trifluoroacetic anhydride T291
C_3H_7Cl	2-chloropropane C264	$C_4F_6O_3$	octafluoro-2-butene O5
C_3H_7ClO	2-chloropropanol C267	C_4F_8	octafluoroisobutene O6
C_3H_7ClO	3-chloropropanol C268	C_4F_8	cobalt hydrocarbonyl C374
C_3H_7ClO	1-chloro-2-propanol C266	C_4HCoO_4	fumaryl chloride F117
$C_3H_7ClO_2$	3-chloro-1,2-propanediol C265	$C_4H_2Cl_2O_2$	maleic anhydride M13
C_3H_7N	allylamine A74	$C_4H_2O_3$	5-fluorouracil F79
C_3H_7N	2-methylaziridine M158	$C_4H_3FN_2O_2$	5-chloro-2-methyl-4-isothiazolinone
C_3H_7NO	dimethylformamide D416	$C_4H_4CaCl_3NOS$	calcium chloride complex C213
C_3H_7NO	N-methylacetamide M150		5-chloro-2-methyl-4-isothiazolinone C212
$C_3H_7NO_2$	1-nitropropane N138	C_4H_4ClNOS	copper tartrate C444
$C_3H_7NO_2$	2-nitropropane N139		N-nitrosobis(2,2,2-trifluoroethyl)-amine N145
$C_3H_7NO_2$	urethane U13	$C_4H_4CuO_6$	succinonitrile S130
$C_3H_7NO_3$	propyl nitrate P334	$C_4H_4F_6N_2O$	2-thiouracil T145
$C_3H_7NO_3$	isopropyl nitrate I129		maleic hydrazide M14
$C_3H_7NO_3$	DL-serine S24	$C_4H_4N_2$	uracil U8
$C_3H_7N_3O_2$	1-nitroso-1-ethylurea N158	$C_4H_4N_2OS$	furan F123
$C_3H_7N_3O_3$	1-(2-hydroxyethyl)-1-nitrosourea H111	$C_4H_4N_2O_2$	2(5H)-furanone F124
C_3H_8	propane P292	$C_4H_4N_2O_2$	diketene D363
$C_3H_8NO_5P$	glyphosate G40	C_4H_4O	cyclobutane-1,3-dione C499
$C_3H_8N_2O$	N-ethyl-N-formylhydrazine E124	$C_4H_4O_2$	succinic anhydride S129
$C_3H_8N_2O$	N-nitroso-N-methylethylamine N161	$C_4H_4O_2$	maleic acid M12
		$C_4H_4O_3$	fumaric acid F115
C_3H_8O	ethyl methyl ether E147	$C_4H_4O_4$	iron(II) fumarate I72
C_3H_8O	1-propanol P296	$C_4H_4O_4Fe$	thiophene T139
C_3H_8O	2-propanol P297	C_4H_4S	chloroprene C262
$C_3H_8OS_2$	dimercaprol D369	C_4H_5Cl	methacryloyl chloride M109
$C_3H_8O_2$	2-methoxyethanol M134	C_4H_5ClO	methyl 2-chloroacrylate M187
$C_3H_8O_2$	dimethoxymethane D382	$C_4H_5ClO_2$	allyl chloroformate A79
$C_3H_8O_2$	propylene glycol P327	$C_4H_5ClO_2$	2,3,4-trichloro-1-butene T244
$C_3H_8O_3$	glycerol G25	$C_4H_5Cl_3$	trichlorobutylene oxide T245
$C_3H_8O_3S$	ethyl methanesulfonate E146	$C_4H_5Cl_3O$	methacrylonitrile M108
C_3H_8S	1-propanethiol P294	C_4H_5N	pyrrole P366
$C_3H_9BO_3$	trimethyl borate T308	C_4H_5N	hymexazol H121
C_3H_9ClSn	trimethyltin chloride T327	$C_4H_5NO_2$	allyl isothiocyanate A87
C_3H_9ClSi	chlorotrimethylsilane C304	C_4H_5NS	1-nitroso-5,6-dihydrouracil N150
C_3H_9N	trimethylamine T303	$C_4H_5N_3O_3$	1-butyne B281
C_3H_9N	isopropylamine I121	C_4H_6	1,3-butadiene B197
C_3H_9N	propylamine P323		
C_3H_9NO	2-(methylamino)ethanol M155		

C ₄ H ₆	crotonylene C469	C ₄ H ₇ Cl	4-chloro-1-butene C179
C ₄ H ₆ As ₆ Cu ₄ O	Paris Green P15	C ₄ H ₇ Cl	1-chloro-2-butene C176
C ₄ H ₆ BaO ₄	barium acetate B6	C ₄ H ₇ Cl	3-chloro-2-methylpropene C216
C ₄ H ₆ CdO ₄	cadmium acetate C3	C ₄ H ₇ Cl	3-chloro-1-butene C178
C ₄ H ₆ CIN	4-chlorobutyronitrile C180	C ₄ H ₇ Cl	2-chloro-2-butene C177
C ₄ H ₆ CINO	4-chloro-3-hydroxybutanenitrile C203	C ₄ H ₇ ClO	1-chloro-2-methylpropene C215
C ₄ H ₆ CINO	1-azetidinecarbonyl chloride A262	C ₄ H ₇ ClO	2-chloroethyl vinyl ether C199
C ₄ H ₆ Cl ₂	1,4-dichloro-2-butene D200	C ₄ H ₇ ClO ₂	butyryl chloride B290
C ₄ H ₆ Cl ₂	<i>trans</i> -1,4-dichloro-2-butene D201	C ₄ H ₇ ClO ₂	methyl 2-chloropropionate M189
C ₄ H ₆ Cl ₂ O ₂	2,3-dichloro- <i>p</i> -dioxane D207	C ₄ H ₇ ClO ₂	isopropyl chloroformate I124
C ₄ H ₆ Cl ₂ O ₂	<i>trans</i> -2,3-dichloro- <i>p</i> -dioxane D208	C ₄ H ₇ ClO ₂	ethyl chloroacetate E106
C ₄ H ₆ CuO ₄	copper acetate C430	C ₄ H ₇ Cl ₂ O ₄ P	propyl chloroformate P326
C ₄ H ₆ HgO ₄	mercury(II) acetate M65	C ₄ H ₇ N	dichlorvos D258
C ₄ H ₆ MnN ₂ S ₄	maneb M21	C ₄ H ₇ N	butyronitrile B289
C ₄ H ₆ N ₂	1-methylimidazole M236	C ₄ H ₇ NO	isobutyronitrile I99
C ₄ H ₆ N ₂ Na ₂ S ₄	nabam N1	C ₄ H ₇ NO	acetone cyanohydrin A18
C ₄ H ₆ N ₂ O ₂	muscimol M356	C ₄ H ₇ NO	propyl isocyanate P333
C ₄ H ₆ N ₂ S	methimazole M122	C ₄ H ₇ NO	methacrylamide M105
C ₄ H ₆ N ₂ S ₄ Zn	zineb Z18	C ₄ H ₇ NO ₂	<i>N</i> -(hydroxymethyl)acrylamide H113
C ₄ H ₆ O	methyl vinyl ketone M318	C ₄ H ₇ NO ₄	iminodiacetic acid I11
C ₄ H ₆ O	methacrolein M103	C ₄ H ₇ NaOS ₂	proxan-sodium P343
C ₄ H ₆ O	crotonaldehyde C467	C ₄ H ₈	<i>trans</i> -2-butene B217
C ₄ H ₆ O	divinyl ether D581	C ₄ H ₈	1-butene B215
C ₄ H ₆ O ₂	γ-butyrolactone B288	C ₄ H ₈	<i>cis</i> -2-butene B216
C ₄ H ₆ O ₂	vinyl acetate V26	C ₄ H ₈	isobutene I86
C ₄ H ₆ O ₂	2,3-butanedione B209	C ₄ H ₈ Cl ₂ O	bis(2-chloroethyl) ether B120
C ₄ H ₆ O ₂	β-butyrolactone B287	C ₄ H ₈ Cl ₂ S	mustard gas M359
C ₄ H ₆ O ₂	<i>meso</i> -1,2:3,4-diepoxybutane D280	C ₄ H ₈ Cl ₃ O ₄ P	trichlorfon T225
C ₄ H ₆ O ₂	1,4-butyne diol B282	C ₄ H ₈ N ₂	2-dimethylaminoacetonitrile D385
C ₄ H ₆ O ₂	methacrylic acid M106	C ₄ H ₈ N ₂ O	<i>N</i> -nitrosopyrrolidine N174
C ₄ H ₆ O ₂	methyl acrylate M153	C ₄ H ₈ N ₂ O	acetaldehyde formylmethylhydrazone A8
C ₄ H ₆ O ₂	crotonic acid C468	C ₄ H ₈ N ₂ O ₂	<i>N</i> -nitrosomorpholine N166
(C ₄ H ₆ O ₂) _n	polyvinyl acetate P233	C ₄ H ₈ N ₂ O ₃	<i>N</i> -nitroso- <i>N</i> -methylurethane N164
C ₄ H ₆ O ₂	allyl formate A83	C ₄ H ₈ N ₂ O ₃	methylazoxymethanol acetate M160
C ₄ H ₆ O ₂	DL-1,2:3,4-diepoxybutane D279		allylthiourea A93
C ₄ H ₆ O ₂	1,2:3,4-diepoxybutane D278		dinitrosopiperazine D496
C ₄ H ₆ O ₂ S	3-sulfolene S144		methyl ethyl ketone M220
C ₄ H ₆ O ₂ S	vinyl sulfone V38		<i>trans</i> -2-buten-1-ol B218
C ₄ H ₆ O ₂ S ₄	dimexano D463		3-buten-1-ol B219
C ₄ H ₆ O ₃	acetic anhydride A13		3-buten-2-ol B220
C ₄ H ₆ O ₄	diacetyl peroxide D66		butyraldehyde B283
C ₄ H ₆ O ₄	succinic acid S128		tetrahydrofuran T72
C ₄ H ₆ O ₄ Pb	lead acetate L12		1,2-epoxybutane E36
C ₄ H ₆ O ₄ S	thiodiglycolic acid T130		crotyl alcohol C470
C ₄ H ₆ O ₄ Zn	zinc acetate Z3		isobutyraldehyde I97
C ₄ H ₆ O ₅	malic acid M15		2-methyl-2-propen-1-ol M289
C ₄ H ₆ O ₆	L-tartaric acid T9		ethyl vinyl ether E181
C ₄ H ₆ O ₆	DL-tartaric acid T8		isopropyl formate I126
C ₄ H ₆ O ₆ U	uranyl acetate U10		
C ₄ H ₇ BrO ₂	ethyl bromoacetate E102		
C ₄ H ₇ Br ₂ Cl ₂ O ₄ P	naled N3		

C ₄ H ₈ O ₂	1,3-dioxane D529	C ₄ H ₁₀ O	1-butanol B212
C ₄ H ₈ O ₂	glycidyl methyl ether G32	C ₄ H ₁₀ O	<i>tert</i> -butanol B214
C ₄ H ₈ O ₂	isobutyric acid I98	C ₄ H ₁₀ O	2-butanol B213
C ₄ H ₈ O ₂	ethyl acetate E87	C ₄ H ₁₀ O	diethyl ether D304
C ₄ H ₈ O ₂	butyric acid B285	C ₄ H ₁₀ O	methyl propyl ether M291
C ₄ H ₈ O ₂	1,4-dioxane D530	C ₄ H ₁₀ O ₂	1,1-dimethoxyethane D380
C ₄ H ₈ O ₂	methyl propionate M290	C ₄ H ₁₀ O ₂	2,3-butanediol B205
C ₄ H ₈ O ₂	methoxyacetone M131	C ₄ H ₁₀ O ₂	1,2-dimethoxyethane D381
C ₄ H ₈ O ₂	aldol A63	C ₄ H ₁₀ O ₂	1,4-butanediol B204
C ₄ H ₈ O ₂	propyl formate P331	C ₄ H ₁₀ O ₂	1,3-butanediol B203
C ₄ H ₈ O ₂ S	sulfolane S143	C ₄ H ₁₀ O ₂	<i>tert</i> -butyl hydroperoxide B261
C ₄ H ₈ O ₃	methyl lactate M247	C ₄ H ₁₀ O ₂	1,2-butanediol B202
C ₄ H ₈ O ₃	ethylene glycol acetate E117	C ₄ H ₁₀ O ₂	2-ethoxyethanol E76
C ₄ H ₈ O ₃ S	1,4-butane sultone B210	C ₄ H ₁₀ O ₂	1-methoxy-2-propanol M147
C ₄ H ₈ S	tetrahydrothiophene T77	C ₄ H ₁₀ O ₂	methoxypropanol M146
C ₄ H ₉ Br	2-bromobutane B165	C ₄ H ₁₀ O ₂ S	2,2'-thiodiethanol T129
C ₄ H ₉ Br	1-bromobutane B164	C ₄ H ₁₀ O ₃	diethylene glycol D301
C ₄ H ₉ Cl	butyl chloride B251	C ₄ H ₁₀ O ₃	trimethyl orthoformate T313
C ₄ H ₉ Cl	<i>tert</i> -butyl chloride B253	C ₄ H ₁₀ O ₄ S	diethyl sulfate D317
C ₄ H ₉ Cl	<i>sec</i> -butyl chloride B252	C ₄ H ₁₀ O ₈ Pb ₃	lead subacetate L29
C ₄ H ₉ I	1-iodobutane I46	C ₄ H ₁₀ S	ethyl sulfide E172
C ₄ H ₉ I	2-iodobutane I47	C ₄ H ₁₀ S	1-butanethiol B211
C ₄ H ₉ I	1-iodo-2-methylpropane I53	C ₄ H ₁₀ Zn	diethylzinc D322
C ₄ H ₉ I	2-iodo-2-methylpropane I54	C ₄ H ₁₁ N	<i>N,N</i> -dimethylethylamine D414
C ₄ H ₉ N	pyrrolidine P367	C ₄ H ₁₁ N	butylamine B239
C ₄ H ₉ NO	butyraldoxime B284	C ₄ H ₁₁ N	diethylamine D288
C ₄ H ₉ NO	<i>N,N</i> -dimethylacetamide D383	C ₄ H ₁₁ N	<i>tert</i> -butylamine B241
C ₄ H ₉ NO	morpholine M353	C ₄ H ₁₁ N	<i>sec</i> -butylamine B240
C ₄ H ₉ NO	methyl ethyl ketone oxime M221	C ₄ H ₁₁ N	isobutylamine I89
C ₄ H ₉ NO ₂	1-nitrobutane N101	C ₄ H ₁₁ NO	2-dimethylaminoethanol D388
C ₄ H ₉ NO ₂	<i>n</i> -propyl carbamate P325	C ₄ H ₁₁ NO ₂	diethanolamine D281
C ₄ H ₉ NO ₃	butyl nitrate B268	C ₄ H ₁₁ NO ₂	2-(2-aminoethoxy)ethanol A127
C ₄ H ₉ NO ₃	L-threonine T152	C ₄ H ₁₁ NO ₃	tris(hydroxymethyl)aminomethane T356
C ₄ H ₉ NO ₅	tris(hydroxymethyl)nitromethane T357	C ₄ H ₁₁ NO ₈ P ₂	glyphosine G41
C ₄ H ₉ N ₃ S	acetone thiosemicarbazide A19	C ₄ H ₁₁ PO ₄	butyl acid phosphate B237
C ₄ H ₉ N ₅ O ₃	1-propyl-3-nitro-3-nitrosoguanidine P335	C ₄ H ₁₂ ClN ₅	metformin hydrochloride M100
C ₄ H ₁₀	butane B199	C ₄ H ₁₂ ClO ₄ P	tetrakis(hydroxymethyl)-phosphonium chloride T79
C ₄ H ₁₀	isobutane I84	C ₄ H ₁₂ FN ₂ OP	dimefox D367
C ₄ H ₁₀ BF ₃ O	boron trifluoride diethyl etherate B148	C ₄ H ₁₂ N ₂	1,2-diethylhydrazine D306
C ₄ H ₁₀ ClO ₂ PS	diethyl chlorothiophosphate D300	C ₄ H ₁₂ N ₂	1,4-butanediamine B201
C ₄ H ₁₀ ClO ₃ P	diethyl chlorophosphate D299	C ₄ H ₁₂ N ₂	1,3-butanediamine B200
C ₄ H ₁₀ FO ₂ P	sarin S8	C ₄ H ₁₂ N ₂ O ₆	ammonium tartrate A188
C ₄ H ₁₀ Hg	diethylmercury D308	C ₄ H ₁₂ O ₄ Si	tetramethyl orthosilicate T91
C ₄ H ₁₀ NO ₃ PS	acephate A5	C ₄ H ₁₂ Pb	tetramethyllead T90
C ₄ H ₁₀ N ₂	piperazine P200	C ₄ H ₁₂ Si	tetramethylsilane T93
C ₄ H ₁₀ N ₂ O	<i>N</i> -nitrosodiethylamine N149	C ₄ H ₁₃ NO	tetramethylammonium hydroxide T86
C ₄ H ₁₀ N ₂ O ₃	<i>N</i> -nitrosodiethanolamine N148	C ₄ H ₁₃ N ₃	diethylenetriamine D303
C ₄ H ₁₀ N ₂ S	trimethylthiourea T326	C ₄ H ₁₄ CuN ₄	cupriethylenediamine C477
C ₄ H ₁₀ O	isobutanol I85	C ₄ NiO ₄	nickel tetracarbonyl N51

C ₅ Cl ₆	hexachlorocyclopentadiene H35	C ₅ H ₈ O ₂	isopropenyl acetate I118
C ₅ FeO ₅	iron pentacarbonyl I75	C ₅ H ₈ O ₂	acetylacetone A22
C ₅ H ₂ Cl ₄	1,2,3,4-tetrachloro-1,3-cyclopentadiene T47	C ₅ H ₈ O ₂	ethyl acrylate E89
C ₅ H ₄ CIN	3-chloropyridine C280	C ₅ H ₈ O ₂	glutaraldehyde G21
C ₅ H ₄ CIN	2-chloropyridine C279	C ₅ H ₈ O ₂	methyl methacrylate M252
C ₅ H ₄ N ₂ O ₃	4-nitropyridine 1-oxide N144	C ₅ H ₈ O ₂	allyl acetate A72
C ₅ H ₄ N ₂ O ₄	orotic acid O34	C ₅ H ₈ O ₂	γ-valerolactone V3
C ₅ H ₄ N ₄	purine P346	C ₅ H ₈ O ₂	pivalolactone P211
C ₅ H ₄ N ₄ O	allopurinol A70	C ₅ H ₈ O ₂	tiglic acid T157
C ₅ H ₄ N ₄ O ₂	xanthine X2	C ₅ H ₈ O ₂	2,3-pentanedione P40
C ₅ H ₄ N ₄ O ₃	uric acid U14	C ₅ H ₈ O ₃	levulinic acid L40
C ₅ H ₄ N ₄ S	6-mercaptopurine M63	C ₅ H ₈ O ₃	methyl acetoacetate M152
C ₅ H ₄ O ₂	2-furaldehyde F120	C ₅ H ₉ Cl	3-chloro-2-methyl-1-butene C211
C ₅ H ₄ O ₂	3-furaldehyde F121	C ₅ H ₉ Cl	1-chloro-2-methyl-2-butene C210
C ₅ H ₅ AsCl ₂	ethyldichloroarsine E112	C ₅ H ₉ ClO	1-chloro-3-pentanone C235
C ₅ H ₅ Cl ₃ N ₂ OS	etridiazole E185	C ₅ H ₉ ClO	5-chloro-2-pentanone C236
C ₅ H ₅ N	pyridine P357	C ₅ H ₉ ClO ₂	butyl chloroformate B254
C ₅ H ₅ NO ₂	methyl 2-cyanoacrylate M196	C ₅ H ₉ ClO ₂	ethyl 2-chloropropionate E108
C ₅ H ₅ N ₃ O	pyrazinamide P348	C ₅ H ₉ Cl ₂ N ₃ O ₂	1,3-bis(chloroethyl)-1-nitrosoarea B121
C ₅ H ₅ N ₃ O ₃ S	acinitrazole A31	C ₅ H ₉ N	isovaleronitrile I142
C ₅ H ₅ N ₅ O	guanine G50	C ₅ H ₉ NO	butyl isocyanate B264
C ₅ H ₆	1,3-cyclopentadiene C528	C ₅ H ₉ NO	N-methylpyrrolidone M298
C ₅ H ₆ Cl ₂ N ₂ O ₂	1,3-dichloro-5,5-dimethylhydantoin D205	C ₅ H ₉ NO	2-piperidinone P202
C ₅ H ₆ N ₂	2-methylpyrazine M293	C ₅ H ₉ NO ₂	L-proline P284
C ₅ H ₆ N ₂	2-aminopyridine A151	C ₅ H ₉ NO ₄ S	carbocysteine C67
C ₅ H ₆ N ₂	4-aminopyridine A153	C ₅ H ₁₀	cyclopentane C522
C ₅ H ₆ N ₂	3-aminopyridine A152	C ₅ H ₁₀	3-methyl-1-butene M175
C ₅ H ₆ N ₂ OS	6-methyl-2-thiouracil M312	C ₅ H ₁₀	amylene A200
C ₅ H ₆ N ₂ O ₂	thymine T153	C ₅ H ₁₀	1-pentene P43
C ₅ H ₆ O	2-methylfuran M228	C ₅ H ₁₀ Br ₂	1,5-dibromopentane D136
C ₅ H ₆ O ₂	furfuryl alcohol F127	C ₅ H ₁₀ Br ₂ O ₂	dibromoneopentyl glycol D134
C ₅ H ₆ O ₄	itaconic acid I144	C ₅ H ₁₀ CIN	1-chloropiperidine C260
C ₅ H ₇ NO	furfurylamine F128	C ₅ H ₁₀ CINO	diethylcarbamoyl chloride D296
C ₅ H ₇ NO ₂	ethyl cyanoacetate E110	C ₅ H ₁₀ Cl ₂	1,5-dichloropentane D234
C ₅ H ₇ N ₃ O ₄	azaserine A260	C ₅ H ₁₀ Cl ₂ O ₂	bis(2-chloroethoxy)methane B118
C ₅ H ₈	cyclopentene C527	C ₅ H ₁₀ HgO ₃	2-methoxyethylmercury acetate M137
C ₅ H ₈	isoprene I115	C ₅ H ₁₀ NNaS ₂	dithiocarb D575
C ₅ H ₈	1,3-pentadiene P34	C ₅ H ₁₀ NO ₂ S ₂ K	potassium bis(2-hydroxyethyl)-dithiocarbamate P240
C ₅ H ₈ Br ₄	pentaerythrityl tetrabromide P37	C ₅ H ₁₀ N ₂	3-(dimethylamino)propionitrile D391
C ₅ H ₈ Cl ₂ O	3,3-bis(chloromethyl)oxetane B124	C ₅ H ₁₀ N ₂ O	nitrosopiperidine N172
C ₅ H ₈ N ₂	1,2-dimethylimidazole D424	C ₅ H ₁₀ N ₂ O ₂ S	methomyl M126
C ₅ H ₈ N ₂ S ₄ Znn(t)	propineb P307	C ₅ H ₁₀ N ₂ S ₂	dazomet D24
C ₅ H ₈ O	2,3-dihydro-4-methylfuran D345	C ₅ H ₁₀ N ₄ O ₂	dinitrosomopiperazine D494
C ₅ H ₈ O	dihdropyran D346	C ₅ H ₁₀ N ₆ O ₂	N,N'-dinitrosopentamethyl-enetetramine D495
C ₅ H ₈ O	3-methyl-3-buten-2-one M179	C ₅ H ₁₀ O	allyl ethyl ether A82
C ₅ H ₈ O	2-methyl-3-buten-2-ol M182	C ₅ H ₁₀ O	isovaleraldehyde I140
C ₅ H ₈ O	6-oxabicyclo[3.1.0]hexane O43	C ₅ H ₁₀ O	2-methyltetrahydrofuran M308
C ₅ H ₈ O	cyclopentanone C525		
C ₅ H ₈ O	3-penten-2-one P44		

C ₅ H ₁₀ O	3-methyl-2-buten-1-ol M176	C ₅ H ₁₂ O	3-methyl-1-butanol M174
C ₅ H ₁₀ O	diethyl ketone D307	C ₅ H ₁₂ O	2-methyl-2-butanol M173
C ₅ H ₁₀ O	2-methyl-3-buten-2-ol M178	C ₅ H ₁₂ O ₂	1-ethoxy-2-propanol E84
C ₅ H ₁₀ O	valeraldehyde V1	C ₅ H ₁₂ O ₂	diethoxymethane D286
C ₅ H ₁₀ O	3-methyl-3-buten-1-ol M177	C ₅ H ₁₂ O ₂	2-isopropoxyethanol I119
C ₅ H ₁₀ O	cyclopentanol C524	C ₅ H ₁₂ O ₂	2-propoxyethanol P316
C ₅ H ₁₀ O	methyl propyl ketone M292	C ₅ H ₁₂ O ₂	neopentyl glycol N40
C ₅ H ₁₀ O	methyl isopropyl ketone M244	C ₅ H ₁₂ O ₃	2-(2-methoxyethoxy)ethanol M135
C ₅ H ₁₀ O	2-methylbutyraldehyde M183		pentaerythritol P35
C ₅ H ₁₀ O ₂	isobutyl formate I90	C ₅ H ₁₂ O ₄	xylitol X13
C ₅ H ₁₀ O ₂	butyl formate B258	C ₅ H ₁₂ O ₅	amyl mercaptan A201
C ₅ H ₁₀ O ₂	isopropyl acetate I120	C ₅ H ₁₂ S	chlormequat chloride C141
C ₅ H ₁₀ O ₂	methyl isobutyrate M242	C ₅ H ₁₃ Cl ₂ N	<i>N</i> -methylbutylamine M180
C ₅ H ₁₀ O ₂	ethyl propionate E165	C ₅ H ₁₃ N	pentylamine P47
C ₅ H ₁₀ O ₂	isovaleric acid I141	C ₅ H ₁₃ N	1-dimethylamino-2-propanol D390
C ₅ H ₁₀ O ₂	tetrahydrofurfuryl alcohol T74	C ₅ H ₁₃ NO	methyldiethanolamine M206
C ₅ H ₁₀ O ₂	propyl acetate P322		<i>O,O</i> -diethyl <i>S</i> -methyl dithiophosphate D310
C ₅ H ₁₀ O ₂	valeric acid V2	C ₅ H ₁₃ NO ₂	choline C326
(C ₅ H ₁₀ O ₂) _x	poloxamer P218	C ₅ H ₁₃ O ₂ PS ₂	3-dimethylaminopropylamine D392
C ₅ H ₁₀ O ₃	diethyl carbonate D298		glufosinate-ammonium G18
C ₅ H ₁₀ O ₃	(-)-ethyl lactate E142	C ₅ H ₁₄ NO	chloranil C115
C ₅ H ₁₀ O ₃	ethyl lactate E141	C ₅ H ₁₄ N ₂	quintozene Q12
C ₅ H ₁₀ O ₃	2-methoxyethyl acetate M136		sodium pentachlorophenolate S82
C ₅ H ₁₀ O ₅	D-lyxose L68	C ₅ H ₁₅ N ₂ O ₄ P	hexachlorobenzene H33
C ₅ H ₁₀ O ₅	L-xylose X15	C ₆ Cl ₄ O ₂	tecnazene T14
C ₅ H ₁₀ O ₅	D-xylose X14	C ₆ Cl ₅ NO ₂	pentachlorobenzene P27
C ₅ H ₁₁ Br	1-bromo-3-methylbutane B179	C ₆ Cl ₅ NaO	pentachlorophenol P30
C ₅ H ₁₁ Cl	amyl chloride A198	C ₆ Cl ₆	2,4,6-trichloronitrobenzene T254
C ₅ H ₁₁ Cl ₂ N	mechlorethamine M38	C ₆ HCl ₄ NO ₂	1,2,4,5-tetrachlorobenzene T46
C ₅ H ₁₁ Cl ₂ NO	mechlorethamine <i>N</i> -oxide M39	C ₆ HCl ₅	1,2,3,4-tetrachlorobenzene T44
C ₅ H ₁₁ Cl ₃ Si	amyltrichlorosilane A206	C ₆ HCl ₅ O	1,2,3,5-tetrachlorobenzene T45
C ₅ H ₁₁ N	piperidine P201	C ₆ H ₂ Cl ₃ NO ₂	2,3,4,5-tetrachlorophenol T54
C ₅ H ₁₁ NO	<i>N</i> -methylmorpholine M255	C ₆ H ₂ Cl ₄	2,3,5,6-tetrachlorophenol T56
C ₅ H ₁₁ NO	tetrahydrofurfurylamine T75	C ₆ H ₂ Cl ₄	2,3,4,6-tetrachlorophenol T55
C ₅ H ₁₁ NO ₂	L-valine V6	C ₆ H ₂ Cl ₄ O	2,4,6-trifluoronitrobenzene T293
C ₅ H ₁₁ NO ₂	DL-valine V5	C ₆ H ₂ Cl ₄ O	2,6-dibromo-4-chlorophenol D127
C ₅ H ₁₁ NO ₂	D-valine V4	C ₆ H ₂ F ₃ NO ₂	2,4,6-tribromophenol T207
C ₅ H ₁₁ NO ₂	isoamyl nitrite I81	C ₆ H ₃ Br ₂ ClO	1-chloro-2,4-dinitrobenzene C194
C ₅ H ₁₁ NO ₂ S	D-methionine M124	C ₆ H ₃ Br ₃ O	2-chloro-1,3-dinitrobenzene C195
C ₅ H ₁₁ NO ₃	amyl nitrate A202	C ₆ H ₃ ClN ₂ O ₄	clopyralid C364
C ₅ H ₁₁ N ₂ O ₂ P	Tabun T2	C ₆ H ₃ Cl ₂ NO ₂	3,5-dichloronitrobenzene D231
C ₅ H ₁₂	neopentane N39	C ₆ H ₃ Cl ₂ NO ₂	2,5-dichloronitrobenzene D229
C ₅ H ₁₂	2-methylbutane M172	C ₆ H ₃ Cl ₂ NO ₂	2,3-dichloronitrobenzene D227
C ₅ H ₁₂	pentane P39	C ₆ H ₃ Cl ₂ NO ₂	2,4-dichloronitrobenzene D228
C ₅ H ₁₂ ClO ₂ PS ₂	chlormephos C140	C ₆ H ₃ Cl ₂ NO ₂	3,4-dichloronitrobenzene D230
C ₅ H ₁₂ NO ₃ PS ₂	dimethoate D376	C ₆ H ₃ Cl ₂ NO ₃	2,4-dichloro-6-nitrophenol D233
C ₅ H ₁₂ NO ₄ PS	omethoate O32	C ₆ H ₃ Cl ₃	1,2,4-trichlorobenzene T242
C ₅ H ₁₂ N ₂ S	1,3-diethylthiourea D318	C ₆ H ₃ Cl ₃	1,2,3-trichlorobenzene T241
C ₅ H ₁₂ O	1-ethoxypropane E82		
C ₅ H ₁₂ O	2-ethoxypropane E83		
C ₅ H ₁₂ O	methyl <i>tert</i> -butyl ether M181		
C ₅ H ₁₂ O	1-pentanol P41		

$C_6H_3Cl_3$	trichlorobenzene (technical mixture) T240	$C_6H_4N_2O_5$	dinitrophenol D484
$C_6H_3Cl_3$	1,3,5-trichlorobenzene T243	$C_6H_4N_2O_5Na$	2,4-dinitrophenolate sodium D490
$C_6H_3Cl_3N_2O_2$	picloram P182	$C_6H_4N_4O_3S$	2-amino-5-(5-nitro-2-furyl)-1,3,4-thiadiazole A137
$C_6H_3Cl_3O$	2,4,5-trichlorophenol T258	$C_6H_4O_2$	<i>o</i> -benzoquinone B73
$C_6H_3Cl_3O$	2,3,4-trichlorophenol T255	$C_6H_4O_2$	<i>p</i> -benzoquinone B74
$C_6H_3Cl_3O$	2,3,5-trichlorophenol T256	$C_6H_5AsCl_2$	phenyldichloroarsine P98
$C_6H_3Cl_3O$	2,3,6-trichlorophenol T257	C_6H_5Br	bromobenzene B161
$C_6H_3Cl_3O$	2,4,6-trichlorophenol T259	C_6H_5Cl	chlorobenzene C163
$C_6H_3Cl_3O$	3,4,5-trichlorophenol T260	C_6H_5ClHg	phenylmercuric chloride P118
$C_6H_3Cl_4N$	nitrapyrin N66	$C_6H_5ClN_2O_2$	4-chloro-2-nitroaniline C221
$C_6H_3Cl_4NO_2S$	2,3,5,6-tetrachloro-4-(methylsulfonyl)pyridine T52	$C_6H_5ClN_2O_2$	2-chloro-4-nitroaniline C220
$C_6H_3Cl_5Si$	dichlorophenyltrichlorosilane D243	C_6H_5ClO	2-chlorophenol C239
$C_6H_3FN_2O_4$	2,4-dinitrofluorobenzene D476	C_6H_5ClO	3-chlorophenol C240
$C_6H_3N_3O_6$	1,3,5-trinitrobenzene T329	C_6H_5ClO	4-chlorophenol C241
$C_6H_3N_3O_7$	picric acid P187	$C_6H_5ClO_2S$	benzenesulfonyl chloride B48
$C_6H_4BrNO_2$	2-bromonitrobenzene B180	$C_6H_5Cl_2N$	2,5-dichloroaniline D180
$C_6H_4BrNO_2$	4-bromonitrobenzene B181	$C_6H_5Cl_2N$	2,6-dichloroaniline D181
$C_6H_4Br_2$	1,4-dibromobenzene D124	$C_6H_5Cl_2N$	3,5-dichloroaniline D183
$C_6H_4Br_2$	dibromobenzene D123	$C_6H_5Cl_2N$	2,4-dichloroaniline D179
$C_6H_4ClNO_2$	2-chloronitrobenzene C222	$C_6H_5Cl_2N$	2,3-dichloroaniline D178
$C_6H_4ClNO_2$	4-chloronitrobenzene C224	$C_6H_5Cl_2N$	3,4-dichloroaniline D182
$C_6H_4ClNO_2$	3-chloronitrobenzene C223	$C_6H_5Cl_2P$	dichlorophenylphosphine D242
$C_6H_4ClNO_3$	5-chloro-2-nitrophenol C230	$C_6H_5Cl_3Si$	phenyltrichlorosilane P137
$C_6H_4ClNO_3$	4-chloro-2-nitrophenol C229	C_6H_5F	fluorobenzene F61
$C_6H_4ClNO_3$	2-chloro-4-nitrophenol C227	C_6H_5FO	3-fluorophenol F69
$C_6H_4ClNO_3$	3-chloro-4-nitrophenol C228	C_6H_5FO	4-fluorophenol F70
$C_6H_4Cl_2$	1,4-dichlorobenzene D190	C_6H_5FO	2-fluorophenol F68
$C_6H_4Cl_2$	1,3-dichlorobenzene D189	$C_6H_5F_2N$	2,4-difluoroaniline D329
$C_6H_4Cl_2$	1,2-dichlorobenzene D188	C_6H_5I	iodobenzene I45
$C_6H_4Cl_2N_2O_2$	dicloran D260	C_6H_5IO	4-iodophenol I55
$C_6H_4Cl_2O$	2,6-dichlorophenol D238	$C_6H_5NO_2$	nitrobenzene N82
$C_6H_4Cl_2O$	2,3-dichlorophenol D236	$C_6H_5NO_2$	4-nitrosophenol N170
$C_6H_4Cl_2O$	2,4-dichlorophenol D237	$C_6H_5NO_2$	nicotinic acid N57
$C_6H_4Cl_3N$	2,3,4-trichloroaniline T231	$C_6H_5NO_3$	3-nitrophenol N131
$C_6H_4Cl_3N$	3,4,5-trichloroaniline T234	$C_6H_5NO_3$	2-nitrophenol N130
$C_6H_4Cl_3N$	2,4,6-trichloroaniline T233	$C_6H_5NO_3$	4-nitrophenol N132
$C_6H_4Cl_3N$	2,4,5-trichloroaniline T232	$C_6H_5NO_5S$	2-nitrobenzenesulfonic acid N83
$C_6H_4N_2$	4-cyanopyridine C489	$C_6H_5NO_5S$	3-nitrobenzenesulfonic acid N84
$C_6H_4N_2$	3-cyanopyridine C488	$C_6H_5NO_5S$	4-nitrobenzenesulfonic acid N85
$C_6H_4N_2$	2-cyanopyridine C487	$C_6H_5N_3$	benzotriazole B78
$C_6H_4N_2O_4$	1,3-dinitrobenzene D471	$C_6H_5N_3O_4$	2,4-dinitroaniline D467
$C_6H_4N_2O_4$	1,2-dinitrobenzene D470	$C_6H_5N_3O_4$	3,5-dinitroaniline D469
$C_6H_4N_2O_4$	1,4-dinitrobenzene D472	$C_6H_5N_3O_4$	2,6-dinitroaniline D468
$C_6H_4N_2O_4$	dinitrobenzene (mixed) D473	$C_6H_5N_3O_5$	2-amino-4,6-dinitrophenol A126
$C_6H_4N_2O_5$	2,3-dinitrophenol D485	$C_6H_5N_5O$	pterin P345
$C_6H_4N_2O_5$	2,6-dinitrophenol D488	C_6H_5NaO	sodium phenolate S85
$C_6H_4N_2O_5$	2,5-dinitrophenol D487	C_6H_6	benzene B47
$C_6H_4N_2O_5$	3,4-dinitrophenol D489	C_6H_6BrN	4-bromoaniline B160
$C_6H_4N_2O_5$	2,4-dinitrophenol D486	$C_6H_6Br_2N_2$	2-bromo-2-(bromomethyl)-pentanedinitrile B163
		C_6H_6ClN	<i>N</i> -chloroaniline C157

C ₆ H ₆ ClN	2-chloroaniline C154	C ₆ H ₇ NO	3-aminophenol A143
C ₆ H ₆ ClN	3-chloroaniline C155	C ₆ H ₇ NO	4-aminophenol A144
C ₆ H ₆ ClN	4-chloroaniline C156	C ₆ H ₇ NO ₃ S	metanilic acid M97
C ₆ H ₆ ClNO	2-amino-4-chlorophenol A124	C ₆ H ₇ NO ₃ S	sulfanilic acid S138
C ₆ H ₆ Cl ₂ N ₂	2,6-dichloro- <i>p</i> -phenylenediamine D240	C ₆ H ₇ NO ₃ S	aniline-2-sulfonic acid A211
C ₆ H ₆ Cl ₆	ε-lindane L48	C ₆ H ₇ N ₃ O	isoniazid I109
C ₆ H ₆ Cl ₆	γ-HCH H10	C ₆ H ₇ N ₃ O ₂	4-nitrophenylhydrazine N136
C ₆ H ₆ Cl ₆	HCH H9	C ₆ H ₇ N ₃ O ₂	2-nitrophenylhydrazine N135
C ₆ H ₆ Cl ₈ O	bis(2,3,3,3-tetrachloropropyl) ether B136	C ₆ H ₇ N ₃ O ₂	4-nitro- <i>o</i> -phenylenediamine N134
C ₆ H ₆ FN	4-fluoroaniline F60	C ₆ H ₇ N ₃ O ₂	2-nitro- <i>p</i> -phenylenediamine N133
C ₆ H ₆ FN	2-fluoroaniline F58	C ₆ H ₇ N ₃ O ₂	cellulose nitrate C98
C ₆ H ₆ FN	3-fluoroaniline F59	C ₆ H ₇ N ₃ O ₂	6-methoxyguanine M139
C ₆ H ₆ HgO	phenylmercuric hydroxide P119	C ₆ H ₇ N ₃ O ₂	sodium sorbate S91
C ₆ H ₆ IN	4-iodoaniline I44	C ₆ H ₇ N ₃ O ₂	sodium ascorbate S46
C ₆ H ₆ IN	3-iodoaniline I43	C ₆ H ₇ N ₃ O ₂	phenylphosphine P129
C ₆ H ₆ N ₂ O	nicotinamide N53	C ₆ H ₇ N ₃ O ₂	aniline hydrochloride A210
C ₆ H ₆ N ₂ O ₂	<i>p</i> -benzoquinone dioxime B75	C ₆ H ₇ N ₃ O ₂	clomethiazole C360
C ₆ H ₆ N ₂ O ₂	2-nitroaniline N74	(C ₆ H ₇ N ₃ O ₁₁) _n	trisodium nitrilotriacetate, monohydrate T358
C ₆ H ₆ N ₂ O ₂	3-nitroaniline N75	C ₆ H ₇ N ₅ O	2,3-dimethylpyrazine D451
C ₆ H ₆ N ₂ O ₂	4-nitroaniline N76	C ₆ H ₇ NaO ₂	2,5-dimethylpyrazine D452
C ₆ H ₆ N ₂ O ₃	2-amino-4-nitrophenol A138	C ₆ H ₇ NaO ₆	2,6-dimethylpyrazine D454
C ₆ H ₆ N ₂ O ₃	2-amino-5-nitrophenol A139	C ₆ H ₇ P	phenylhydrazine P108
C ₆ H ₆ N ₂ O ₃	4-amino-2-nitrophenol A140	C ₆ H ₈ ClN	<i>o</i> -phenylenediamine P102
C ₆ H ₆ N ₄ O ₃ S	niridazole N62	C ₆ H ₈ ClNS	adiponitrile A49
C ₆ H ₆ N ₄ O ₄	2,4-dinitrophenylhydrazine D491	C ₆ H ₈ ClNS	2,5(<i>or</i> 2,6)-dimethylpyrazine D453
C ₆ H ₆ N ₄ O ₄	nitrofurazone N116	C ₆ H ₈ NO ₇ Na ₃	<i>p</i> -phenylenediamine P103
C ₆ H ₆ N ₄ O ₇	ammonium picrate A182		<i>m</i> -phenylenediamine P101
C ₆ H ₆ O	phenol P80		2,4-diaminophenol D81
C ₆ H ₆ O ₂	catechol C95		benzenesulfonyl hydrazide B49
C ₆ H ₆ O ₂	resorcinol R5		nithiazide N63
C ₆ H ₆ O ₂	hydroquinone H107		5,5-dimethyl-2(5 <i>H</i>)-furanone D417
C ₆ H ₆ O ₃	pyrogallol P363		sorbic acid S102
C ₆ H ₆ S	benzenethiol B50		acrolein dimer A36
C ₆ H ₇ AsNNaO ₃	sodium arsanilate S43		maple lactone M31
C ₆ H ₇ AsO ₃	phenylarsonic acid P93		parascorbic acid P12
C ₆ H ₇ BHgO ₃	phenylmercuric borate P117		glycidyl acrylate G29
C ₆ H ₇ ClN ₂	2-chloro- <i>p</i> -phenylenediamine C242		dimethyl maleate D426
C ₆ H ₇ ClN ₂	4-chloro- <i>m</i> -phenylenediamine C244		ascorbic acid A248
C ₆ H ₇ ClN ₂	4-chloro- <i>o</i> -phenylenediamine C245		citric acid C352
C ₆ H ₇ Cl ₂ N	2-picoyl chloride hydrochloride P186		phenylhydrazine hydrochloride P109
C ₆ H ₇ KO ₂	potassium sorbate P263		2-chloro- <i>p</i> -phenylenediamine sulfate C243
C ₆ H ₇ N	aniline A209		3-cyclohexenyltrichlorosilane C512
C ₆ H ₇ N	4-picoline P185		chromium(III) acetate C332
C ₆ H ₇ N	3-picoline P184		<i>N</i> -vinyl-2-pyrrolidinone V37
C ₆ H ₇ N	2-picoline P183		nitrilotriacetic acid N70
C ₆ H ₇ NO	2-aminophenol A142		3,3'-iminodipropionitrile I13
			metronidazole M327

$(C_6H_5ON)_n$	polyvinylpyrrolidone P236	$C_6H_{12}Cl_3N$	tris(2-chloroethyl)amine T349
C_6H_{10}	cyclohexene C511	$C_6H_{12}Cl_3O_4P$	tris(2-chloroethyl) phosphate T350
$C_6H_{10}Cl_2N_2$	<i>p</i> -phenylenediamine	$C_6H_{12}NNaO_3S$	sodium cyclamate S59
	dihydrochloride P105	$C_6H_{12}NO_3PS_2$	fosthietan F109
$C_6H_{10}Cl_2N_2$	<i>m</i> -phenylenediamine	$C_6H_{12}NO_4PS_2$	formothion F105
	dihydrochloride P104	$C_6H_{12}N_2O_2$	<i>N</i> -nitroso-2,6-dimethylmorpholine N153
$C_6H_{10}Cl_2N_2O$	2,4-diaminophenol dihydrochloride D82		daminozide D21
$C_6H_{10}N_3O_2$	cupferron C476	$C_6H_{12}N_2O_3$	lead dimethyldithiocarbamate L18
$C_6H_{10}N_6$	cyromazine C545	$C_6H_{12}N_2PbS_4$	monothiourea M348
$C_6H_{10}N_6O$	dacarbazine D17	$C_6H_{12}N_2S_3$	thiram T147
$C_6H_{10}O$	cyclohexanone C509	$C_6H_{12}N_2S_4$	ziram Z19
$C_6H_{10}O$	diallyl ether D71	$C_6H_{12}N_2S_4Zn$	tris(1-aziridinyl)phosphine oxide T346
$C_6H_{10}O$	mesityl oxide M91	$C_6H_{12}N_3OP$	tris(1-aziridinyl)phosphine sulfide T347
$C_6H_{10}O_2$	2,5-hexanedione H62		hexamethylenetetramine H57
$C_6H_{10}O_2$	3-methyl-2,4-pentanedione M276	$C_6H_{12}N_3PS$	menazon M50
$C_6H_{10}O_2$	allyl glycidyl ether A84	$C_6H_{12}N_4$	cyclohexanol C508
$C_6H_{10}O_2$	ethyl methacrylate E145	$C_6H_{12}N_5O_2PS_2$	3-hexanone H68
$C_6H_{10}O_2$	vinyl butyrate V29	$C_6H_{12}O$	1-hexen-3-ol H71
$C_6H_{10}O_2$	(<i>E</i>)-ethyl crotonate E109	$C_6H_{12}O$	(<i>E</i>)-2-hexen-1-ol H72
$C_6H_{10}O_2S_4$	dixan D582	$C_6H_{12}O$	(<i>E</i>)-3-hexen-1-ol H73
$C_6H_{10}O_3$	2-hydroxypropyl acrylate H116	$C_6H_{12}O$	hexanal H59
$C_6H_{10}O_3$	ethyl acetoacetate E88	$C_6H_{12}O$	1,2-epoxyhexane E38
$C_6H_{10}O_3$	diglycidyl ether D337	$C_6H_{12}O$	butyl vinyl ether B280
$C_6H_{10}O_3$	propionic anhydride P311	$C_6H_{12}O$	(<i>Z</i>)-3-hexen-1-ol H74
$C_6H_{10}O_4$	dipropionyl peroxide D552	$C_6H_{12}O$	methyl isobutyl ketone M241
$C_6H_{10}O_4$	isosorbide I137	$C_6H_{12}O$	2-methylvaleraldehyde M316
$C_6H_{10}O_4$	diethyl oxalate D312	$C_6H_{12}O$	2-ethylbutyraldehyde E104
$C_6H_{10}O_4$	adipic acid A48	$C_6H_{12}O$	2-hexanone H67
$C_6H_{10}O_4S_2$	dimethipin D374	$C_6H_{12}O$	isobutyl vinyl ether I96
$(C_6H_{10}O_5)_n$	cellulose C97	$C_6H_{12}O$	pinacolone P192
$(C_6H_{10}O_5)_n$	starch S110	$C_6H_{12}O$	hexanoic acid H64
$C_6H_{11}AuO_5S$	aurothioglucose A255	$C_6H_{12}O_2$	diacetone alcohol D65
$C_6H_{11}Cl_3O_3$	1,2,3-tris(chloromethoxy)propane T351	$C_6H_{12}O_2$	<i>tert</i> -butyl acetate B235
	diallylamine D70	$C_6H_{12}O_2$	ethyl butyrate E105
$C_6H_{11}N$	caprolactam C55	$C_6H_{12}O_2$	<i>sec</i> -butyl acetate B234
$C_6H_{11}NO$	nitrocyclohexane N110	$C_6H_{12}O_2$	butyl acetate B233
$C_6H_{11}NO_2$	3-nitro-3-hexene N123	$C_6H_{12}O_2$	methyl isovalerate M246
$C_6H_{11}NO_2$	methidathion M121	$C_6H_{12}O_2$	ethyl isobutyrate E139
$C_6H_{11}N_2O_4PS_3$	trimethylolpropane phosphite T310	$C_6H_{12}O_2$	isobutyl acetate I87
$C_6H_{11}O_3P$	mercury gluconate M74	$C_6H_{12}O_2$	propylene glycol allyl ether P328
$C_6H_{11}O_7Hg$	methylcyclopentane M204	$C_6H_{12}O_2$	glycidyl isopropyl ether G30
C_6H_{12}	1-hexene H70	$C_6H_{12}O_3$	2-methoxypropanol acetate M149
C_6H_{12}	2-methyl-1-pentene M282	$C_6H_{12}O_3$	paraldehyde P9
C_6H_{12}	cyclohexane C507	$C_6H_{12}O_3$	<i>tert</i> -butyl peracetate B270
C_6H_{12}	4-methyl-2-pentene M285	$C_6H_{12}O_3$	1-methoxy-2-propanol acetate M148
C_6H_{12}	2-methyl-2-pentene M283	$C_6H_{12}O_3$	1-ethoxyethyl acetate E78
C_6H_{12}	4-methyl-1-pentene M284	$C_6H_{12}O_3$	2-ethoxyethyl acetate E79
$C_6H_{12}Cl_2O$	dichloroisopropyl ether D221	$C_6H_{12}O_3$	solketal S101
$C_6H_{12}Cl_2O$	DCIP D26		

$C_6H_{12}O_3$	2,5-tetrahydrofuran dimethanol T73	$C_6H_{14}O_8S_2$	treosulfan T195
$C_6H_{12}O_5$	D-fucose F114	$C_6H_{14}S$	1-hexanethiol H63
$C_6H_{12}O_6$	D-mannose M30	$C_6H_{15}BO_3$	ethyl borate E101
$C_6H_{12}O_6$	D-glucose G17	$C_6H_{15}N$	1,3-dimethylbutylamine D404
$C_6H_{12}O_6$	inositol I37	$C_6H_{15}N$	triethylamine T278
$C_6H_{12}O_6$	α -glucose G16	$C_6H_{15}N$	diisopropylamine D358
$C_6H_{12}O_6$	D-fructose F111	$C_6H_{15}N$	dipropylamine D554
$C_6H_{12}S$	cyclohexyl mercaptan C518	$C_6H_{15}NO$	2-diethylaminoethanol D289
$C_6H_{12}S_2$	allyl propyl disulfide A92	$C_6H_{15}NO_2$	diisopropanolamine D356
$C_6H_{13}Cl_2N$	HN1 H82	$C_6H_{15}NO_3$	triethanolamine T276
$C_6H_{13}Cl_3Si$	hexyltrichlorosilane H79	$C_6H_{15}NSO_4$	cyclohexylamine sulfate C515
$C_6H_{13}N$	hexamethyleneimine H56	$C_6H_{15}N_2O_2Cl$	carbachol chloride C60
$C_6H_{13}N$	cyclohexylamine C514	$C_6H_{15}N_3$	<i>N</i> -aminoethylpiperazine A129
$C_6H_{13}N$	1-methylpiperidine M288	$C_6H_{15}O_2PS_3$	thiometon T134
$C_6H_{13}NO$	4-ethylmorpholine E152	$C_6H_{15}O_3P$	triethyl phosphite T288
$C_6H_{13}NO_2$	D-isoleucine I108	$C_6H_{15}O_3PS_2$	demeton-methyl D50
$C_6H_{13}NO_2$	DL-leucine L36	$C_6H_{15}O_3PS_2$	demeton-S-methyl D54
$C_6H_{13}NO_3S$	cyclamic acid C495	$C_6H_{15}O_3PS_2$	demeton-O-methyl D52
$C_6H_{13}N_3O_2$	1-amyl-1-nitrosourea A203	$C_6H_{15}O_4P$	triethyl phosphate T287
C_6H_{14}	3-methylpentane M274	$C_6H_{15}O_4PS_2$	oxydemeton-methyl O57
C_6H_{14}	2-methylpentane M273	$C_6H_{15}O_5PS_2$	demeton-S-methyl sulfone D55
C_6H_{14}	hexane H60	$C_6H_{16}N_2$	<i>N,N</i> -diethylethylenediamine D305
$C_6H_{14}FO_3P$	isofluorophate I106	$C_6H_{16}N_2$	hexamethylenediamine H54
$C_6H_{14}NO_3PS_2$	ethoate-methyl E71	$C_6H_{16}N_2$	<i>N,N,N',N'</i> -tetramethyl- ethylenediamine T89
$C_6H_{14}NO_4P$	dimethyl morpholino- phosphoramidate D432	$C_6H_{16}O_2Si$	diethoxydimethylsilane D284
$C_6H_{14}N_2O$	<i>N</i> -nitrosodipropylamine N156	$C_6H_{16}O_3Si$	triethoxysilane T277
$C_6H_{14}N_2O$	<i>N</i> -nitrosodiisopropylamine N152	$C_6H_{17}N_3$	norspermidine N208
$C_6H_{14}N_2O_3$	<i>N</i> -nitrosodiisopropanolamine N151	$C_6H_{18}AlO_9P_3$	fosetyl-aluminium F108
$C_6H_{14}O$	2-hexanol H66	$C_6H_{18}N_3OP$	hexamethylphosphoramidate H58
$C_6H_{14}O$	1-hexanol H65	$C_6H_{18}N_4$	triethylenetetramine T284
$C_6H_{14}O$	dipropyl ether D557	$C_6H_{18}OSi_2$	hexamethyldisiloxane H53
$C_6H_{14}O$	3-methyl-3-pentanol M279	$C_6H_{18}O_{24}P_6$	phytic acid P180
$C_6H_{14}O$	2-methyl-3-pentanol M278	$C_6H_{19}NSi_2$	hexamethyldisilazane H52
$C_6H_{14}O$	2-methyl-1-pentanol M277	$C_6H_{20}N_2O_{12}P_4$	EDTPA E11
$C_6H_{14}O$	diisopropyl ether D359	$C_7H_2Cl_6$	1,2,3,4,7,7'-hexachloro- norbornadiene H40
$C_6H_{14}O$	2-ethyl-1-butanol E103	$C_7H_3Br_2NO$	bromoxynil B189
$C_6H_{14}O$	butyl ethyl ether B257	$C_7H_3ClF_3NO_2$	4-chloro-3-nitrobenzotrifluoride C225
$C_6H_{14}O$	4-methyl-1-pentanol M280	$C_7H_3Cl_2N$	3,5-dichlorobenzonitrile D196
$C_6H_{14}O$	4-methyl-2-pentanol M281	$C_7H_3Cl_2N$	dichlobenil D166
$C_6H_{14}O_2$	acetal A6	$C_7H_3Cl_2NO$	3,4-dichlorophenyl isocyanate D241
$C_6H_{14}O_2$	2-butoxyethanol B226	$C_7H_3Cl_3O_2$	2,3,6-TBA T10
$C_6H_{14}O_2$	1,2-diethoxyethane D285	$C_7H_3Cl_4NO_3$	2,3,5,6-tetrachloro-4-nitroanisole T53
$C_6H_{14}O_2$	2-methyl-2,4-pentanediol M275		2,4-dichlorobenzotrichloride D197
$C_6H_{14}O_3$	dipropylene glycol D555		2,3,4,5,6-pentachloroanisole P26
$C_6H_{14}O_3$	diglyme D338		ioxynil I59
$C_6H_{14}O_4$	triethylene glycol T280		4-chlorobenzotrifluoride C170
$C_6H_{14}O_6$	D-mannitol M28		3-chlorobenzotrifluoride C169
$C_6H_{14}O_6$	D-sorbitol S104		
$C_6H_{14}O_6S_2$	busulfan B195		

$C_7H_4ClF_3$	2-chlorobenzotrifluoride C168	$C_7H_6ClNO_2$	4-nitrobenzyl chloride N97
C_7H_4ClNO	4-chlorophenyl isocyanate C248	$C_7H_6ClNO_2$	4-chloro-2-nitrotoluene C232
C_7H_4ClNO	2-chlorophenyl isocyanate C246	$C_7H_6ClN_3O_4S_2$	chlorothiazide C287
C_7H_4ClNO	3-chlorophenyl isocyanate C247	$C_7H_6Cl_2$	2,4-dichlorotoluene D253
$C_7H_4Cl_2O$	2,6-dichlorobenzaldehyde D187	$C_7H_6Cl_2$	3,4-dichlorotoluene D255
$C_7H_4Cl_2O_2$	3,4-dichlorobenzoic acid D195	$C_7H_6Cl_2$	2-chlorobenzyl chloride C172
$C_7H_4Cl_2O_2$	2,6-dichlorobenzoic acid D194	$C_7H_6Cl_2$	4-chlorobenzyl chloride C174
$C_7H_4Cl_3NO_3$	triclopyr T271	$C_7H_6Cl_2$	3-chlorobenzyl chloride C173
$C_7H_4Cl_4$	4-chlorobenzotrichloride C167	$C_7H_6Cl_2$	benzylidene chloride B98
$C_7H_4Cl_4$	2-chlorobenzotrichloride C166	$C_7H_6Cl_2$	2,6-dichlorotoluene D254
$C_7H_4F_3NO_2$	3-nitrobenzotrifluoride N94	$C_7H_6Cl_2O$	2,6-dichlorobenzyl alcohol D198
$C_7H_4F_3NO_2$	2-nitrobenzotrifluoride N93	$C_7H_6Cl_2O$	2,3-dichloroanisole D184
$C_7H_4F_3NO_2$	4-nitrobenzotrifluoride N95	$C_7H_6Cl_2O$	3,5-dichloroanisole D186
$C_7H_4HgO_3$	mercury salicylate M84	$C_7H_6Cl_2O$	2,6-dichloroanisole D185
$C_7H_4N_2O_2$	2-nitrobenzonitrile N90	$C_7H_6F_3N$	3-aminobenzotrifluoride A118
$C_7H_4N_2O_2$	4-nitrobenzonitrile N92	$C_7H_6N_2$	indazole I22
$C_7H_4N_2O_2$	3-nitrobenzonitrile N91	$C_7H_6N_2$	benzimidazole B53
$C_7H_5BiO_6$	bismuth subgallate B131	$C_7H_6N_2O_4$	2,5-dinitrotoluene D500
$C_7H_5ClN_2O$	zoxazolamine Z25	$C_7H_6N_2O_4$	4-nitroanthranilic acid N80
C_7H_5ClO	benzoyl chloride B82	$C_7H_6N_2O_4$	dinitrotoluene D497
C_7H_5ClO	2-chlorobenzaldehyde C161	$C_7H_6N_2O_4$	2,6-dinitrotoluene D501
C_7H_5ClO	3-chlorobenzaldehyde C162	$C_7H_6N_2O_4$	3,5-dinitrotoluene D503
$C_7H_5ClO_2$	2-chlorobenzoic acid C165	$C_7H_6N_2O_4$	2,3-dinitrotoluene D498
$C_7H_5ClO_2$	phenyl chloroformate P97	$C_7H_6N_2O_4$	3,4-dinitrotoluene D502
$C_7H_5ClO_3$	3-chloroperbenzoic acid C237	$C_7H_6N_2O_4$	2,4-dinitrotoluene D499
$C_7H_5Cl_2FN_2O_3$	fluroxypyr F88	$C_7H_6N_2O_5$	4,6-dinitro- <i>o</i> -cresol D475
$C_7H_5Cl_2NO_2$	chloramben C110	$C_7H_6N_2O_5$	2,6-dinitro- <i>p</i> -cresol D474
$C_7H_5Cl_2NS$	chlorthiamid C319	$C_7H_6N_2S$	2-mercaptobenzimidazole M60
$C_7H_5Cl_3$	benzotrichloride B79	$C_7H_6N_4O_3S$	2-hydrazino-4-(5-nitro-2-furyl)thiazole H92
$C_7H_5Cl_3$	2,4,5-trichlorotoluene T268		2,4-diamino-6-(5-nitro-2-furanyl)-s-triazine D80
$C_7H_5Cl_3O$	2,3,4-trichloroanisole T235	C_7H_6O	benzaldehyde B40
$C_7H_5Cl_3O$	2,4,5-trichloroanisole T238	$C_7H_6O_2$	benzoic acid B63
$C_7H_5Cl_3O$	2,4,6-trichloroanisole T239	$C_7H_6O_2$	β -furylacrolein F131
$C_7H_5Cl_3O$	2,3,5-trichloroanisole T236	$C_7H_6O_2$	1-butoxy-2-propanol B231
$C_7H_5Cl_3O$	2,3,6-trichloroanisole T237	$C_7H_6O_2$	salicylaldehyde S4
$C_7H_5F_3$	benzotrifluoride B80	$C_7H_6O_2$	salicylic acid S6
C_7H_5N	benzonitrile B68	$C_7H_6O_3$	patulin P16
C_7H_5NO	phenyl isocyanate P113	$C_7H_6O_3$	benzyl bromide B92
$C_7H_5NO_3$	3-nitrobenzaldehyde N81	$C_7H_6O_4$	3-chlorotoluene C289
$C_7H_5NO_3S$	saccharin S1	C_7H_7Br	2-chlorotoluene C288
$C_7H_5NO_4$	2-nitrobenzoic acid N87	C_7H_7Cl	benzyl chloride B95
$C_7H_5NO_4$	3-nitrobenzoic acid N88	C_7H_7Cl	4-chlorotoluene C290
$C_7H_5NO_4$	4-nitrobenzoic acid N89	C_7H_7Cl	chloramine T C113
$C_7H_5NO_5$	1,2-benzisothiazolin-3-one B54	C_7H_7Cl	(2-chlorophenyl)thiourea C251
C_7H_5NS	benzothiazole B76	$C_7H_7ClNNaO_2S$	4-chloro- <i>m</i> -cresol C183
C_7H_5NS	phenyl isothiocyanate P115	C_7H_7ClO	6-chloro- <i>o</i> -cresol C187
$C_7H_5NS_2$	2-mercaptobenzothiazole M61	C_7H_7ClO	3-chloro- <i>o</i> -cresol C181
$C_7H_5N_3O_2$	5(6)-nitrobenzimidazole N86	C_7H_7ClO	5-chloro- <i>o</i> -cresol C185
$C_7H_5N_3O_6$	2,4,6-trinitrotoluene T331	C_7H_7ClO	3-chloro- <i>p</i> -cresol C182
$C_7H_5N_5O_8$	nitramine N65	C_7H_7ClO	4-chloro- <i>o</i> -cresol C184
C_7H_6ClNO	4-chloroformanilide C202		
$C_7H_6ClNO_2$	6-chloro-2-nitrotoluene C233		

C ₇ H ₇ ClO	6-chloro- <i>m</i> -cresol C186	C ₇ H ₈ N ₂ O ₂	2-methyl-5-nitroaniline M260
C ₇ H ₇ ClO ₂ S	<i>p</i> -toluenesulfonyl chloride T180	C ₇ H ₈ N ₂ O ₃	2-methoxy-5-nitroaniline M142
C ₇ H ₇ Cl ₂ NO	clopidol C363	C ₇ H ₈ N ₂ O ₃	2-methoxy-4-nitroaniline M141
C ₇ H ₇ Cl ₃ NO ₃ PS	chlorpyrifos-methyl C314	C ₇ H ₈ N ₂ O ₃	4-methoxy-2-nitroaniline M143
C ₇ H ₇ F	4-fluorotoluene F77	C ₇ H ₈ N ₂ S	phenylthiourea P136
C ₇ H ₇ F	2-fluorotoluene F76	C ₇ H ₈ N ₄ O ₂	theobromine T109
C ₇ H ₇ N	2-vinylpyridine V35	C ₇ H ₈ N ₄ O ₂	theophylline T110
C ₇ H ₇ N	4-vinylpyridine V36	C ₇ H ₈ O	benzyl alcohol B89
C ₇ H ₇ NO	benzamide B42	C ₇ H ₈ O	<i>o</i> -cresol C458
C ₇ H ₇ NO ₂	3-nitrotoluene N180	C ₇ H ₈ O	anisole A216
C ₇ H ₇ NO ₂	4-aminobenzoic acid A117	C ₇ H ₈ O	cresol C456
C ₇ H ₇ NO ₂	2-nitrotoluene N179	C ₇ H ₈ O	<i>p</i> -cresol C459
C ₇ H ₇ NO ₂	4-nitrotoluene N181	C ₇ H ₈ O	<i>m</i> -cresol C457
C ₇ H ₇ NO ₂	3-aminobenzoic acid A116	C ₇ H ₈ O ₂	4-methoxyphenol M144
C ₇ H ₇ NO ₂	2-aminobenzoic acid A115	C ₇ H ₈ O ₃ S	<i>p</i> -toluenesulfonic acid T179
C ₇ H ₇ NO ₂	salicylamide S5	C ₇ H ₉ Cl ₂ N	4-chloro- <i>o</i> -toluidine hydrochloride C295
C ₇ H ₇ NO ₃	4-nitro- <i>m</i> -cresol N105		
C ₇ H ₇ NO ₃	4-nitrobenzyl alcohol N96	C ₇ H ₉ N	2-ethylpyridine E166
C ₇ H ₇ NO ₃	6-nitro- <i>o</i> -cresol N108	C ₇ H ₉ N	2,3-lutidine L61
C ₇ H ₇ NO ₃	2-nitro- <i>m</i> -cresol N103	C ₇ H ₉ N	2,4-lutidine L62
C ₇ H ₇ NO ₃	6-nitro- <i>m</i> -cresol N107	C ₇ H ₉ N	2,5-lutidine L63
C ₇ H ₇ NO ₃	2-nitro- <i>p</i> -cresol N104	C ₇ H ₉ N	4-ethylpyridine E168
C ₇ H ₇ NO ₃	5-nitro- <i>o</i> -cresol N106	C ₇ H ₉ N	3-ethylpyridine E167
C ₇ H ₇ NO ₃	3-nitroanisole N78	C ₇ H ₉ N	benzylamine B90
C ₇ H ₇ NO ₃	2-nitroanisole N77	C ₇ H ₉ N	<i>o</i> -toluidine T185
C ₇ H ₇ NO ₃	4-nitroanisole N79	C ₇ H ₉ N	<i>p</i> -toluidine T187
C ₇ H ₇ N ₃	4(<i>or</i> 5)-methylbenzotriazole M164	C ₇ H ₉ N	<i>N</i> -methylaniline M156
C ₇ H ₇ N ₃	1-methylbenzotriazole M163	C ₇ H ₉ N	2,6-lutidine L64
C ₇ H ₇ N ₃	5-methylbenzotriazole M165	C ₇ H ₉ N	<i>m</i> -toluidine T184
C ₇ H ₇ N ₃ O ₂	<i>N</i> -methyl- <i>N</i> ,4-dinitrosoaniline M207	C ₇ H ₉ NO	2-anisidine A213
	toluene T173	C ₇ H ₉ NO	3-anisidine A214
C ₇ H ₈	2,5-norbornadiene N202	C ₇ H ₉ NO	4-anisidine A215
C ₇ H ₈	cycloheptatriene C506	C ₇ H ₉ NO ₂	ammonium benzoate A164
C ₇ H ₈ BrClO ₂	3-bromo-1-chloro-5,5-dimethylhydantoin B169	C ₇ H ₉ NO ₂	<i>N</i> -isopropylmaleimide I127
	6-chloro- <i>o</i> -toluidine C297	C ₇ H ₉ NO ₂	<i>N</i> -ethyl-2-methylmaleimide E148
	5-chloro- <i>o</i> -toluidine C296	C ₇ H ₉ NO ₂ S	<i>p</i> -toluenesulfonamide T178
	3-chloro- <i>p</i> -toluidine C293	C ₇ H ₉ NO ₃	methacryloyloxyethyl isocyanate M110
	4-chloro- <i>o</i> -toluidine C294		phenicarbazide P75
	3-chloro- <i>o</i> -toluidine C292	C ₇ H ₉ N ₃ O	<i>o</i> -toluidine hydrochloride T186
	2-chloro- <i>p</i> -toluidine C291	C ₇ H ₁₀ ClN	crimidine C463
	3-chloro- <i>p</i> -anisidine C158	C ₇ H ₁₀ ClN ₃	3,4-diaminotoluene D92
	hydrochlorothiazide H94	C ₇ H ₁₀ N ₂	2,3-diaminotoluene D86
	dichloromethylphenylsilane D224	C ₇ H ₁₀ N ₂	2,6-diaminotoluene D90
	<i>N</i> -methyl-3-pyridinecarboxamide M297	C ₇ H ₁₀ N ₂	3,5-diaminotoluene D93
	<i>N</i> -nitroso- <i>N</i> -methylaniline N160	C ₇ H ₁₀ N ₂	2,5-diaminotoluene D88
	<i>N</i> -methyl-4-nitroaniline M263	C ₇ H ₁₀ N ₂	2,4-diaminotoluene D87
	2-methyl-4-nitroaniline M259	C ₇ H ₁₀ N ₂ O	2-ethyl-5-methylpyrazine E149
	4-methyl-3-nitroaniline M262	C ₇ H ₁₀ N ₂ OS	2,4-diaminoanisole D73
	4-methyl-2-nitroaniline M261	C ₇ H ₁₀ N ₄ O ₂ S	6-propyl-2-thiouracil P337
		C ₇ H ₁₀ N ₄ O ₃	sulfaguanidine S134
			cymoxanil C541

$C_7H_{10}O$	1,2,3,6-tetrahydrobenzaldehyde T71	$C_7H_{14}O$	methylcyclohexanol M198
$C_7H_{10}O_3$	glycidyl methacrylate G31	$C_7H_{14}O$	3-heptanone H24
$C_7H_{10}O_4$	acrolein diacetate A37	$C_7H_{14}O$	4-heptanone H25
$C_7H_{10}O_5$	shikimic acid S26	$C_7H_{14}O$	2-heptanone H23
$C_7H_{11}NO$	cyclohexyl isocyanate C517	$C_7H_{14}O$	2,4-dimethyl-3-pentanone D447
$C_7H_{11}N_3O_4$	misonidazole M335	$C_7H_{14}O$	5-methyl-2-hexanone M233
$C_7H_{11}N_7S$	aziprotrotyne A265	$C_7H_{14}O_2$	amyl acetate A195
$C_7H_{12}ClN_5$	simazine S37	$C_7H_{14}O_2$	isobutyl propionate I95
$C_7H_{12}Cl_2N_2$	2,6-diaminotoluene dihydrochloride D91	$C_7H_{14}O_2$	<i>tert</i> -butyl glycidyl ether B260
$C_7H_{12}N_2$	<i>N</i> -butylimidazole B263	$C_7H_{14}O_2$	isopropyl butyrate I123
$C_7H_{12}N_2O_4$	<i>N,N'</i> -dimethylol-5,5-dimethyl- hydantoin D446	$C_7H_{14}O_2$	butyl propionate B277
$C_7H_{12}N_2O_4S$	2,5-diaminotoluene sulfate D89	$C_7H_{14}O_2$	2-pentyl acetate P46
$C_7H_{12}N_2O_4S$	2,5-toluenediamine sulfate T174	$C_7H_{14}O_2$	<i>tert</i> -amyl acetate A196
$C_7H_{12}N_2O_5S$	2,4-diaminoanisole sulfate D74	$C_7H_{14}O_2$	4-methoxy-4-methyl-2-pentanone M140
$C_7H_{12}N_4O_3S_2$	ethidimuron E64	$C_7H_{14}O_2$	butyl glycidyl ether B259
$C_7H_{12}O$	2-methylcyclohexanone M203	$C_7H_{14}O_2$	isoamyl acetate I80
$C_7H_{12}O$	methylcyclohexanone M202	$C_7H_{14}O_2$	heptanoic acid H22
$C_7H_{12}O_2$	butyl acrylate B238	$C_7H_{14}O_3$	acrolein diethyl acetal A39
$C_7H_{12}O_2$	isobutyl acrylate I88	$C_7H_{14}O_3$	butyl lactate B266
$C_7H_{12}O_2$	allyl butyrate A77	$C_7H_{15}Cl_2N_2O_2P$	2-propoxyethanol acetate P317
$C_7H_{12}O_3$	2-hydroxypropyl methacrylate H117	$C_7H_{15}Cl_2N_2O_2P$	cyclophosphamide C529
$(C_7H_{12}O_5)_n$	methylcellulose M185	$C_7H_{15}N$	ifosfamide I3
$C_7H_{13}BrN_2O_2$	carbromal C85	C_7H_{16}	1-ethylpiperidine E164
$C_7H_{13}NO_4S_3$	thiocyclam hydrogen oxalate T126	$C_7H_{16}ClN_3O_2S_2$	heptane H20
$C_7H_{13}N_3O_3S$	oxamyl O47	$C_7H_{16}NO_4PS_2$	cartap hydrochloride C92
$C_7H_{13}O_5PS$	methacrifos M102	$C_7H_{16}O_2$	amidithion A110
$C_7H_{13}O_6P$	mevinphos M330	$C_7H_{16}O_3$	butoxypropanol B230
C_7H_{14}	1-heptene H26	$C_7H_{16}O_3$	triethyl orthoformate T286
C_7H_{14}	cycloheptane C505	$C_7H_{16}O_4$	dipropylene glycol methyl ether D556
C_7H_{14}	methylcyclohexane M197	$C_7H_{16}O_4$	triethylene glycol monomethyl ether T283
C_7H_{14}	(<i>Z</i>)-2-heptene H27	$C_7H_{16}S$	1-heptanethiol H21
C_7H_{14}	(<i>Z</i>)-3-heptene H28	$C_7H_{17}O_2PS_3$	phorate P145
$C_7H_{14}NO_3PS_2$	phosfolan P151	$C_7H_{18}N_2$	3-diethylaminopropylamine D290
$C_7H_{14}NO_5P$	monocrotophos M343	$C_7H_{19}N_3$	spermidine S106
$C_7H_{14}NO_5P$	dimethyl (<i>Z</i>)-1-methyl-2-methyl- carbamoylviny phosphate D429	$C_8Cl_4N_2$	chlorothalonil C286
$C_7H_{14}N_2O$	<i>N</i> -nitrosoheptamethyleneimine N159	$C_8Co_2O_8$	cobalt carbonyl C371
$C_7H_{14}N_2O_2S$	butocarboxim B223	$C_8F_{14}O_3$	heptafluorobutyric anhydride H18
$C_7H_{14}N_2O_2S$	aldicarb A62	$C_8H_2Cl_4O_2$	phthalide P174
$C_7H_{14}N_2O_4S$	butoxycarboxim B225	$C_8H_4F_{15}O_2N$	ammonium perfluorooctanoate A180
$C_7H_{14}N_2O_4S$	aldoxycarb A64	$C_8H_4N_2$	isophthalonitrile I114
$C_7H_{14}N_4O_4$	<i>N</i> -(<i>N</i> -methyl- <i>N</i> -nitrosocarbamoyl)- L-ornithine M268	$C_8H_4N_2$	terephthalonitrile T27
$C_7H_{14}O$	3-methylcyclohexanol M200	$C_8H_4N_2S_2$	bitoscanate B138
$C_7H_{14}O$	heptanal H19	$C_8H_4O_3$	phthalic anhydride P173
$C_7H_{14}O$	2-methylcyclohexanol M199	$C_8H_5Cl_2LiO_3$	2,4-D, lithium salt D12
$C_7H_{14}O$	4-methylcyclohexanol M201	$C_8H_5Cl_2O_3Na$	2,4-D, sodium salt D16
		$C_8H_5Cl_3O_2$	chlorfenac C124
		$C_8H_5Cl_3O_3$	2,4,5-T T1

$C_8H_5MnO_3$	manganese cyclopentadienyl tricarbonyl M23	C_8H_8FNO	4'-fluoroacetanilide F54
$C_8H_5NO_2$	phthalimide P175	$C_8H_8HgO_2$	phenylmercuric acetate P116
$C_8H_5NO_2$	isatin I78	$C_8H_8N_2O_2$	<i>N</i> -methyl- <i>N</i> -nitrosobenzamide M267
$C_8H_5N_3O_4S$	<i>N</i> -[4-(5-nitro-2-furyl)-2- thiazolyl]formamide N118	$C_8H_8N_2O_2$	phthalamide P171
C_8H_6BrN	α -bromobenzyl cyanide B162	$C_8H_8N_4O_4$	nifuradene N58
$C_8H_6BrNO_2$	β -bromo- β -nitrostyrene B182	$C_8H_8Na_2O_5$	endothal sodium E23
C_8H_6ClN	7-chloroindole C205	C_8H_8O	styrene oxide S127
$C_8H_6Cl_2O_3$	2,4-D D1	C_8H_8O	acetophenone A21
$C_8H_6Cl_2O_3$	3,4-dichlorophenoxyacetic acid D239	$C_8H_8O_2$	methyl benzoate M161
$C_8H_6Cl_2O_3$	dicamba D165	$C_8H_8O_2$	2-furfurylidene acetone F129
$C_8H_6N_2O_2$	5-nitroindole N126	$C_8H_8O_2$	<i>m</i> -toluic acid T181
$C_8H_6N_4O_4S$	nifurthiazole N59	$C_8H_8O_2$	<i>p</i> -toluic acid T183
$C_8H_6N_4O_5$	nitrofurantoin N115	$C_8H_8O_2$	<i>o</i> -toluic acid T182
C_8H_6O	benzofuran B61	$C_8H_8O_3$	vanillin V17
$C_8H_6O_4$	isophthalic acid I113	$C_8H_8O_3$	methyl salicylate M305
$C_8H_6O_4$	phthalic acid P172	$C_8H_8O_3$	tetrahydrophthalic anhydride T76
$C_8H_6O_4$	terephthalic acid T26	$C_8H_8O_3$	methylparaben M272
C_8H_6S	benzo[<i>b</i>]thiophene B77	$C_8H_8O_3$	DL-mandelic acid M20
C_8H_7Cl	3-chlorostyrene C283	$C_8H_8O_4$	dehydroacetic acid D45
C_8H_7Cl	4-chlorostyrene C284	C_8H_8S	1,3-dihydrobenzo[<i>c</i>]thiophene D343
C_8H_7Cl	2-chlorostyrene C282	$C_8H_9ClNO_5PS$	chlorthion C320
C_8H_7ClO	2-chloroacetophenone C148	$C_8H_9ClN_4$	hydralazine hydrochloride H85
C_8H_7ClO	phenylacetyl chloride P91	C_8H_9ClO	4-chloro-3,5-xylene C306
C_8H_7ClO	4'-chloroacetophenone C149	C_8H_9ClO	6-chloro-3-methylanisole C209
$C_8H_7ClO_2$	4-anisoyl chloride A217	C_8H_9ClO	4-chloro-2-methylanisole C208
$C_8H_7ClO_3$	4-CPA C452	C_8H_9ClO	3-chloro-4-methylanisole C207
$C_8H_7Cl_2NO_3$	2,4-D, amine salt D2	$C_8H_9FN_2O_3$	furaflur F118
$C_8H_7Cl_2NaO_5S$	2,4-DES-sodium D57	C_8H_9N	2-methyl-5-vinylpyridine M319
C_8H_7N	indole I31	C_8H_9NO	acetanilide A11
C_8H_7N	benzyl cyanide B97	$C_8H_9NO_2$	paracetamol P6
C_8H_7N	<i>p</i> -tolunitrile T190	$C_8H_9NO_2$	3-nitro- <i>o</i> -xylene N186
C_8H_7N	<i>o</i> -tolunitrile T189	$C_8H_9NO_2$	4-nitro- <i>m</i> -xylene N187
C_8H_7N	<i>m</i> -tolunitrile T188	$C_8H_9NO_2$	2-nitro- <i>m</i> -xylene N185
C_8H_7NO	<i>p</i> -tolyl isocyanate T192	$C_8H_9NO_2$	4-nitro- <i>o</i> -xylene N188
$C_8H_7NO_3$	4'-nitroacetophenone N73	$C_8H_9O_3PS$	dioxabenzofos D527
C_8H_7NS	2-methylbenzothiazole M162	C_8H_{10}	ethylbenzene E97
$C_8H_7NS_2$	2-(methylthio)benzothiazole M309	C_8H_{10}	<i>p</i> -xylene X7
$C_8H_7N_3O_5$	dinitolmide D465	C_8H_{10}	<i>m</i> -xylene X5
$C_8H_7N_3O_5$	furazolidone F126	C_8H_{10}	<i>o</i> -xylene X6
$C_8H_7NaO_4$	sodium dehydroacetate S60	C_8H_{10}	xylene (mixed isomers) X8
C_8H_8	styrene S126	$C_8H_{10}Br_2O_4$	1,4-bis(bromoacetoxy)-2-butene B114
C_8H_8	cyclooctatetraene C521	$C_8H_{10}ClNO_2$	4-chloro-2,5-dimethoxyaniline C193
$(C_8H_8)_n$	polystyrene P231	$C_8H_{10}Cl_2Si$	dichloroethylphenylsilane D215
$C_8H_8BrCl_2O_3PS$	bromophos B183	$C_8H_{10}K_2O_{15}Sb_2$	antimonyl potassium tartrate hemihydrate A222
$C_8H_8Cl_2IO_3PS$	iodofenphos I50	$C_8H_{10}NO_5PS$	parathion-methyl P14
$C_8H_8Cl_2O$	2,4-dichloro-3,5-xylene D256	$C_8H_{10}N_2O$	<i>N,N</i> -dimethyl-4-nitrosoaniline D445
$C_8H_8Cl_2O_2$	chloroneb C219		
$C_8H_8Cl_3O_3PS$	fenchlorfos F8		

$C_8H_{10}N_2O$	<i>N</i> -nitroso- <i>N</i> -ethylaniline N157	$C_8H_{11}NO$	<i>o</i> -phenetidine P71
$C_8H_{10}N_2O_3S$	<i>N</i> -methyl- <i>N</i> -nitroso- <i>p</i> -toluenesulfonamide M269	$C_8H_{11}NO$	<i>m</i> -cresidine C454
$C_8H_{10}N_2O_4S$	asulam A251	$C_8H_{11}NO_2$	dopamine D595
$C_8H_{10}N_2S$	ethionamide E69	$C_8H_{11}NO_3$	pyridoxine P358
$C_8H_{10}N_2S$	<i>o</i> -tolylthiourea T193	$C_8H_{11}N_5$	1-phenylbiguanide P95
$C_8H_{10}N_3NaO_3S$	fenaminosulf F2	C_8H_{12}	(<i>Z,Z</i>)-1,5-cyclooctadiene C520
$C_8H_{10}N_4O_2$	caffeine C20	C_8H_{12}	1,5-cyclooctadiene C519
$C_8H_{10}O$	4-ethylphenol E162	C_8H_{12}	4-vinyl-1-cyclohexene V31
$C_8H_{10}O$	3-ethylphenol E161	$C_8H_{12}ClNO$	allidochlor A69
$C_8H_{10}O$	2-ethylphenol E160	$C_8H_{12}ClNO_3$	pyridoxine hydrochloride P359
$C_8H_{10}O$	<i>sec</i> -phenethyl alcohol P68	$C_8H_{12}ClN_5O_2$	proglinazine-ethyl P283
$C_8H_{10}O$	phenethyl alcohol P67	$C_8H_{12}NO_2Cl$	2,4-dimethoxyaniline hydrochloride D378
$C_8H_{10}O$	phenetole P73	$C_8H_{12}N_2$	<i>N,N</i> -dimethyl- <i>p</i> -phenylenediamine D448
$C_8H_{10}O$	xynol X9	$C_8H_{12}N_2$	<i>m</i> -xylylenediamine X17
$C_8H_{10}O$	2,4-xynol X10	$C_8H_{12}N_2O_2$	hexamethylene diisocyanate H55
$C_8H_{10}O$	methyl benzyl ether M166	$C_8H_{12}N_4$	azobis(isobutyronitrile) A269
$C_8H_{10}O$	2,5-xynol X11	$C_8H_{12}N_4O_5$	5-azacytidine A257
$C_8H_{10}O$	4-methylanisole M157	$C_8H_{12}O_2$	(±)-4-vinyl-1-cyclohexene diepoxide V32
$C_8H_{10}O$	3,5-xynol X12	$C_8H_{12}O_4$	methacrolein diacetate M104
$C_8H_{10}OS$	3-methyl-4-(methylthio)phenol M254	$C_8H_{12}O_4$	hexahydrophthalic acid H49
$C_8H_{10}O_2$	4-ethyl-1,3-benzenediol E98	$C_8H_{12}O_8Pb$	lead tetraacetate L32
$C_8H_{10}O_2$	veratrole V18	$C_8H_{13}N_2O_3PS$	thionazin T135
$C_8H_{10}O_2$	2-phenoxyethanol P86	C_8H_{14}	2,5-dimethyl-2,4-hexadiene D419
$C_8H_{10}O_3$	methacrylic anhydride M107	C_8H_{14}	1,3-dimethylcyclohexene D410
$C_8H_{10}O_3$	<i>cis</i> -hexahydrophthalic anhydride H50	$C_8H_{14}ClNS_2$	sulfallate S135
$C_8H_{10}O_3S$	methyl <i>p</i> -toluenesulfonate M313	$C_8H_{14}ClN_5$	atrazine A252
$C_8H_{10}O_4$	penicillic acid P21	$C_8H_{14}Cl_3O_5P$	butonate B224
$C_8H_{10}O_5$	endothal E22	$C_8H_{14}N_2O_2S_2$	tirpate T163
$C_8H_{10}O_8$	disuccinoyl peroxide D564	$C_8H_{14}N_2O_4S$	phenelzine sulfate P64
$C_8H_{11}Cl_2NO$	dichlormid D171	$C_8H_{14}N_4OS$	metribuzin M326
$C_8H_{11}Cl_2N_3O_2$	5-bis(2-chloroethyl)aminouracil B119	$C_8H_{14}O$	2-ethyl-2-hexenal E130
$C_8H_{11}Cl_3O_6$	chloralose C109	$C_8H_{14}O$	2-ethylhexenal E129
$C_8H_{11}N$	2,6-dimethylaniline D398	$C_8H_{14}O$	methylheptenone M231
$C_8H_{11}N$	2,5-dimethylaniline D397	$C_8H_{14}O$	6-methyl-5-hepten-2-one M232
$C_8H_{11}N$	2,4-dimethylaniline D396	$C_8H_{14}O_2$	isobutyl methacrylate I92
$C_8H_{11}N$	3,4-dimethylaniline D399	$C_8H_{14}O_2$	butyl methacrylate B267
$C_8H_{11}N$	2,3-dimethylaniline D395	$C_8H_{14}O_2$	allyl isovalerate A88
$C_8H_{11}N$	2-ethylaniline E92	$C_8H_{14}O_3$	butyric anhydride B286
$C_8H_{11}N$	3-ethylaniline E93	$C_8H_{14}O_3$	butyl acetoacetate B236
$C_8H_{11}N$	4-ethylaniline E94	$C_8H_{14}O_4$	ethyl hydrogen adipate E136
$C_8H_{11}N$	3,5-dimethylaniline D400	$C_8H_{14}O_4$	dimethoxane D377
$C_8H_{11}N$	phenethylamine P69	$C_8H_{14}O_4$	ethylene glycol diglycidyl ether E118
$C_8H_{11}N$	<i>N,N</i> -dimethylaniline D394	$C_8H_{14}O_6$	diisopropyl peroxydicarbonate D360
$C_8H_{11}N$	<i>N</i> -ethylaniline E95	$C_8H_{15}NO$	allylisopropylacetamide A86
$C_8H_{11}N$	5-ethyl-2-picoline E163	$C_8H_{15}NO_2$	2-dimethylaminoethyl methacrylate D389
$C_8H_{11}NO$	<i>p</i> -phenetidine P72		
$C_8H_{11}NO$	tyrosamine T375		
$C_8H_{11}NO$	<i>p</i> -cresidine C455		

$C_8H_{15}N_2O_4P$	diethyl 3-methylpyrazol-5-yl phosphate D311	$C_8H_{18}O$	dibutyl ether D145
$C_8H_{15}N_3O_7$	streptozocin S120	$C_8H_{18}O$	2-octanol O14
$C_8H_{15}N_5S$	desmetryn D60	$C_8H_{18}O$	1-octanol O13
$C_8H_{15}N_5S$	simetryn S38	$C_8H_{18}O$	3-octanol O15
$C_8H_{15}NaO_2$	sodium valproate S100	$C_8H_{18}O$	6-methyl-1-heptanol M229
C_8H_{16}	1,2-dimethylcyclohexane D409	$C_8H_{18}OSn$	dibutyltin oxide D164
C_8H_{16}	ethylcyclohexane E111	$C_8H_{18}O_2$	2-ethyl-1,3-hexanediol E126
C_8H_{16}	2,4,4-trimethyl-1-pentene T318	$C_8H_{18}O_2$	di- <i>tert</i> -butyl peroxide D150
C_8H_{16}	2,4,4-trimethylpentene T317	$C_8H_{18}O_2$	2,2,4-trimethyl-1,3-pentanediol T315
$C_8H_{16}NO_3PS_2$	mephosfolan M56	$C_8H_{18}O_3$	2-(2-butoxyethoxy)ethanol B227
$C_8H_{16}NO_4PS_2$	morphothion M354	$C_8H_{18}O_3$	2-ethoxyethyl ether E80
$C_8H_{16}NO_5P$	dicrotophos D263	$C_8H_{18}O_4$	triglyme T296
$C_8H_{16}NO_5P$	dimethyl (Z)-1-methyl-2-dimethyl-carbamoylviny phosphate D428	$C_8H_{18}O_5$	tetraethylene glycol T64
$C_8H_{16}N_2O_7$	cycasin C494	$C_8H_{18}S$	1-octanethiol O10
$C_8H_{16}O$	4-octanone O17	$C_8H_{18}S$	<i>tert</i> -octanethiol O11
$C_8H_{16}O$	2-ethylhexanal E125	$C_8H_{19}N$	di- <i>sec</i> -butylamine D142
$C_8H_{16}O$	octanal O8	$C_8H_{19}N$	diisobutylamine D352
$C_8H_{16}O$	ethyl amyl ketone E91	$C_8H_{19}N$	2-ethylhexylamine E132
$C_8H_{16}O$	2-octanone O16	$C_8H_{19}N$	dibutylamine D141
$C_8H_{16}O$	5-methyl-3-heptanone M230	$C_8H_{19}O_2PS_2$	ethoprophos E74
$C_8H_{16}O$	1-octen-3-ol O18	$C_8H_{19}O_2PS_3$	disulfoton D566
$C_8H_{16}O$	1,2-epoxyoctane E39	$C_8H_{19}O_3PS_2$	demeton-S D53
$C_8H_{16}O_2$	<i>sec</i> -hexyl acetate H77	$C_8H_{19}O_3PS_2$	demeton D49
$C_8H_{16}O_2$	isobutyl isobutyrate I91	$C_8H_{19}O_3PS_2$	demeton-O D51
$C_8H_{16}O_2$	octanoic acid O12	$C_8H_{19}O_3PS_3$	disulfoton sulfoxide D567
$C_8H_{16}O_2$	2-ethylhexanoic acid E127	$C_8H_{19}O_4P$	dibutyl hydrogen phosphate D147
$C_8H_{16}O_2$	butyl butyrate B250	$C_8H_{19}O_5PS_2$	demeton-S sulfone D56
$C_8H_{16}O_2$	valproic acid V8	$C_8H_{20}ClNO_6S_2$	improsfulfan hydrochloride I16
$C_8H_{16}O_2$	pentyl propionate P49	$C_8H_{20}O_4Si$	tetraethyl orthosilicate T67
$C_8H_{16}O_3$	<i>tert</i> -butyl peroxyisobutyrate B272	$C_8H_{20}O_5P_2S_2$	sulfotep S147
$C_8H_{16}O_3$	2-butoxyethyl acetate B229	$C_8H_{20}O_7P_2$	tetraethyl pyrophosphate T68
$C_8H_{16}O_4$	metaldehyde M94	$C_8H_{20}Pb$	tetraethyllead T66
$C_8H_{16}O_4$	methyl ethyl ketone peroxide M222	$C_8H_{20}Sn$	tetraethyltin T69
$C_8H_{16}O_4$	2-(2-ethoxyethoxy)ethanol acetate E77	$C_8H_{23}N_5$	tetraethylenepentamine T65
$C_8H_{16}O_4S_2$	<i>trans</i> -1,2-bis(propylsulfonyl)-ethylene B135	$C_8H_{24}N_4O_3P_2$	schradan S9
$C_8H_{17}Cl_3Sn$	octyltin chloride O24	$C_9H_2Cl_6O_3$	chlorendic anhydride C123
$C_8H_{17}N$	<i>N,N</i> -dimethylcyclohexylamine D411	$C_9H_4Cl_2FNO_2S$	<i>N</i> -(dichlorofluoromethylthio)-phthalimide D217
C_8H_{18}	octane O9	$C_9H_4Cl_3NO_2S$	folpet F97
C_8H_{18}	2,2,4-trimethylpentane T314	$C_9H_4Cl_6O_4$	chlorendic acid C122
$C_8H_{18}Cl_2Sn$	dibutyltin dichloride D161	$C_9H_4Cl_8O$	isobenzan I82
$C_8H_{18}Cl_2Sn$	di- <i>tert</i> -butyltin dichloride D162	$C_9H_4N_2S_3$	thioquinox T142
$C_8H_{18}CrO_4$	<i>tert</i> -butyl chromate B255	$C_9H_4O_5$	trimellitic anhydride T299
$C_8H_{18}NO_4PS_2$	vamidothion V9	$C_9H_5Cl_3N_4$	anilazine A208
$C_8H_{18}N_2O$	<i>N</i> -nitrosodi- <i>sec</i> -butylamine N147	$C_9H_6ClNO_3S$	benazolin B27
$C_8H_{18}N_2O$	<i>N</i> -nitrosodibutylamine N146	$C_9H_6Cl_2N_2O_3$	methazole M120
$C_8H_{18}O$	2-ethylhexanol E128	$C_9H_6Cl_6O_3S$	endosulfan E19
		$C_9H_6Cl_6O_3S$	β -endosulfan E20
		$C_9H_6Cl_6O_4S$	endosulfan sulfate E21
		$C_9H_6N_2O_2$	toluene 2,4-diisocyanate T176
		$C_9H_6N_2O_2$	toluene diisocyanate T175

C ₉ H ₆ N ₂ O ₂	toluene 2,6-diisocyanate T177	C ₉ H ₁₀ N ₂ O	phenidone P76
C ₉ H ₆ N ₂ S ₃	2-(thiocyanatomethylthio)- benzothiazole T125	C ₉ H ₁₀ N ₄ O ₃ S	2-(2,2-dimethylhydrazino)-4-(5- nitro-2-furyl)thiazole D423
C ₉ H ₆ O ₂	coumarin C447	C ₉ H ₁₀ N ₄ S	2-hydrazino-4-(<i>p</i> -amino- phenyl)thiazole H90
C ₉ H ₆ O ₂	1,3-indandione I18	C ₉ H ₁₀ O	5-indanol I19
C ₉ H ₆ O ₄	esculetin E48	C ₉ H ₁₀ O ₂	methyl phenylacetate M286
C ₉ H ₆ O ₄	ninhydrin N60	C ₉ H ₁₀ O ₂	benzyl acetate B88
C ₉ H ₇ Cl ₃ O ₃	fenoprop F14	C ₉ H ₁₀ O ₂	ethyl benzoate E99
C ₉ H ₇ MnO ₃	manganese 2-methylcyclo- pentadienyl tricarbonyl M25	C ₉ H ₁₀ O ₂	glycidyl phenyl ether G35
C ₉ H ₇ N	quinoline Q9	C ₉ H ₁₀ O ₂	ethyl 3-hydroxybenzoate E137
C ₉ H ₇ N	isoquinoline I135	C ₉ H ₁₀ O ₃	ethyl salicylate E169
C ₉ H ₇ NO	2-hydroxyquinoline H118	C ₉ H ₁₀ O ₃	ethylparaben E158
C ₉ H ₇ NO	8-hydroxyquinoline H119	C ₉ H ₁₀ O ₃	glycol salicylate G38
C ₉ H ₇ N ₃ O ₄ S	<i>N</i> -[4-(5-nitro-2-furyl)-2- thiazolyl]acetamide N117	C ₉ H ₁₀ O ₄	cyclopentane-1,2,3,4-tetracarboxylic acid C523
C ₉ H ₇ N ₃ S	tricyclazole T272	C ₉ H ₁₁ BrN ₂ O ₂	metobromuron M322
C ₉ H ₇ N ₇ O ₂ S	azathioprine A261	C ₉ H ₁₁ ClN ₂ O	monuron M350
C ₉ H ₈	indene I23	C ₉ H ₁₁ ClN ₂ O ₂	monolinuron M345
C ₉ H ₈ Cl ₂ O ₃	2,4-D, methyl ester D13	C ₉ H ₁₁ Cl ₂ FN ₂ O ₂ S ₂	dichlofluanid D168
C ₉ H ₈ Cl ₂ O ₃	dichlorprop D257	C ₉ H ₁₁ Cl ₃ NO ₃ PS	chlorpyrifos C313
C ₉ H ₈ Cl ₃ NO ₂ S	captan C59	C ₉ H ₁₁ IN ₂ O ₅	5-iodo-2'-deoxyuridine I48
C ₉ H ₈ N ₂	1-phenylimidazole P111	C ₉ H ₁₁ N	2-methylindoline M239
C ₉ H ₈ N ₄ O ₂ S	2-hydrazino-4-(<i>p</i> - nitrophenyl)thiazole H93	C ₉ H ₁₁ NO	4-(dimethylamino)benzaldehyde D387
C ₉ H ₈ O	1-indanone I20	C ₉ H ₁₁ NO	4'-aminopropiophenone A149
C ₉ H ₈ O	cinnamaldehyde C346	C ₉ H ₁₁ NO ₂	benzocaine B55
C ₉ H ₈ O	2-indanone I21	C ₉ H ₁₁ NO ₂	<i>p</i> -nitrocumene N109
C ₉ H ₈ O ₄	acetylsalicylic acid A28	C ₉ H ₁₁ NO ₂	metolcarb M324
C ₉ H ₈ O ₄	caffeic acid C19	C ₉ H ₁₁ NO ₂	L-phenylalanine P92
C ₉ H ₉ BrO ₂	benzyl bromoacetate B93	C ₉ H ₁₁ NO ₄	levodopa L37
C ₉ H ₉ ClO ₃	MCPA M32	C ₉ H ₁₁ N ₃ O	<i>N</i> -nitrosonornicotine N169
C ₉ H ₉ Cl ₂ NO	propanil P295	C ₉ H ₁₂	5-ethylidene-2-norbornene E138
C ₉ H ₉ HgNaO ₂ S	thiomersal T133	C ₉ H ₁₂	cumene C474
C ₉ H ₉ N	3-methylindole M238	C ₉ H ₁₂	4-ethyltoluene E178
C ₉ H ₉ NO ₃	hippuric acid H81	C ₉ H ₁₂	2-ethyltoluene E176
C ₉ H ₉ NO ₄	glycidyl 4-nitrophenyl ether G33	C ₉ H ₁₂	3-ethyltoluene E177
C ₉ H ₉ NS	phenethyl isothiocyanate P70	C ₉ H ₁₂	1,2,4-trimethylbenzene T307
C ₉ H ₉ N ₃ O ₅	benzthiazuron B87	C ₉ H ₁₂	propylbenzene P324
C ₉ H ₉ N ₃ O ₂	carbendazim C65	C ₉ H ₁₂	5-vinyl-2-norbornene V34
C ₉ H ₉ N ₅	benzoguanamine B62	C ₉ H ₁₂	1,2,3-trimethylbenzene T306
C ₉ H ₁₀	indan I17	C ₉ H ₁₂	mesitylene M90
C ₉ H ₁₀	methylstyrene M306	C ₉ H ₁₂ ClO ₄ P	heptenophos H29
C ₉ H ₁₀	α-methylstyrene M307	C ₉ H ₁₂ NO ₅ PS	fenitrothion F11
C ₉ H ₁₀ BrClN ₂ O ₂	chlorbromuron C116	C ₉ H ₁₂ N ₂ O	fenuron F27
C ₉ H ₁₀ ClNO ₂	3-CPA C451	C ₉ H ₁₂ N ₂ O	<i>N</i> -nitroso- <i>N</i> -(2-phenylethyl)- methylamine N171
C ₉ H ₁₀ ClN ₂ O ₅ PS	azamethiphos A259	C ₉ H ₁₂ N ₂ O	4-ethoxyphenylurea E81
C ₉ H ₁₀ ClN ₅ O ₂	imidacloprid I8	C ₉ H ₁₂ N ₂ O ₂	uridine U15
C ₉ H ₁₀ Cl ₂ N ₂ O	diuron D579	C ₉ H ₁₂ N ₂ O ₆	2,3,6-trimethylphenol T321
C ₉ H ₁₀ Cl ₂ N ₂ O ₂	linuron L50	C ₉ H ₁₂ O	α,4-dimethylbenzyl alcohol D402
C ₉ H ₁₀ NO ₃ PS	cyanophos C486	C ₉ H ₁₂ O	2-phenyl-2-propanol P131
C ₉ H ₁₀ N ₂	2-phenyl-2-imidazoline P112		

C ₉ H ₁₂ O	2,4,6-trimethylphenol T322	C ₉ H ₁₇ NOS	molinate M337
C ₉ H ₁₂ O	4-isopropylphenol I130	C ₉ H ₁₇ N ₅ S	ametryn A109
C ₉ H ₁₂ O	3,4,5-trimethylphenol T323	C ₉ H ₁₈	isopropylcyclohexane I125
C ₉ H ₁₂ O	2,3,5-trimethylphenol T320	C ₉ H ₁₈	tripropylene T343
C ₉ H ₁₂ OS	3,5-dimethyl-4-(methylthio)phenol D431	C ₉ H ₁₈ FeN ₃ S ₆	ferbam F30
C ₉ H ₁₂ O ₂	cumene hydroperoxide C475	C ₉ H ₁₈ N ₂ O ₂ S	thiofanox T131
C ₉ H ₁₂ O ₃ S	ethyl <i>p</i> -toluenesulfonate E179	C ₉ H ₁₈ N ₂ O ₄	meprobamate M57
C ₉ H ₁₃ BrN ₂ O ₂	bromacil B151	C ₉ H ₁₈ N ₃ OP	metepa M99
C ₉ H ₁₃ ClN ₂ O ₂	terbacil T20	C ₉ H ₁₈ O	nonanal N192
C ₉ H ₁₃ ClN ₆	cyanazine C480	C ₉ H ₁₈ O	diisobutyl ketone D353
C ₉ H ₁₃ N	<i>N,N</i> -dimethylbenzylamine D403	C ₉ H ₁₈ O ₂	butyl isovalerate B265
C ₉ H ₁₃ N	2,4,6-trimethylaniline T305	C ₉ H ₁₈ O ₂	amyl butyrate A197
C ₉ H ₁₃ N	amphetamine A193	C ₉ H ₁₈ O ₃	<i>tert</i> -butyl peroxyphthalate B273
C ₉ H ₁₃ N	2,4,5-trimethylaniline T304	C ₉ H ₁₉ Cl ₃ Si	nonyltrichlorosilane N199
C ₉ H ₁₃ NO ₂	phenylephrine P106	C ₉ H ₁₉ NOS	EPTC E40
C ₉ H ₁₃ NO ₃	L-adrenaline A51	C ₉ H ₁₉ N ₃ O ₂	1,3-dibutyl-1-nitrosourea D149
C ₉ H ₁₃ NO ₃	D-adrenaline A50	C ₉ H ₂₀	nonane N193
C ₉ H ₁₃ N ₃ O ₅	cytarabine C546	C ₉ H ₂₀ NO ₃ PS ₂	prothoate P342
C ₉ H ₁₃ O ₄ PS	4-(methylthio)phenyl dimethyl phosphate M311	C ₉ H ₂₀ O	2,6-dimethyl-4-heptanol D418
C ₉ H ₁₃ O ₆ PS	endothion E24	C ₉ H ₂₀ O	1-nonanol N195
C ₉ H ₁₄ ClN	phenyltrimethylammonium chloride P138	C ₉ H ₂₀ S	1-nonanethiol N194
C ₉ H ₁₄ ClNO	norephedrine hydrochloride N203	C ₉ H ₂₁ AlO ₃	aluminium isopropoxide A101
C ₉ H ₁₄ ClN ₅ O ₂	eglinazine-ethyl E12	C ₉ H ₂₁ BO ₃	triisopropyl borate T298
C ₉ H ₁₄ NI	phenyltrimethylammonium iodide P139	C ₉ H ₂₁ ClN ₂ O ₂	propamocarb hydrochloride P291
C ₉ H ₁₄ O	isophorone I110	C ₉ H ₂₁ N	tripropylamine T342
C ₉ H ₁₄ O	phorone P147	C ₉ H ₂₁ NO ₃	triisopropanolamine T297
C ₉ H ₁₄ O ₆	triacetin T196	C ₉ H ₂₁ N ₃	1,3,5-triethylhexahydro- <i>s</i> -triazine T285
C ₉ H ₁₅ BO ₃	triallyl borate T200	C ₉ H ₂₁ N ₃ O ₃	hexahydro-1,3,5-tris(2-hydroxyethyl)- <i>s</i> -triazine H51
C ₉ H ₁₅ Br ₆ O ₄ P	tris(2,3-dibromopropyl) phosphate T352	C ₉ H ₂₁ O ₂ PS ₃	terbufos T22
C ₉ H ₁₅ Cl ₆ O ₄ P	tris(1,3-dichloro-2-propyl) phosphate T353	C ₉ H ₂₂ O ₄ P ₂ S ₄	ethion E68
C ₉ H ₁₅ N	triallylamine T199	C ₉ H ₂₃ NO ₂ Si	(4-aminobutyl)diethoxymethylsilane A122
C ₉ H ₁₆	1-nonyne N200	C ₁₀ Cl ₈	octachloronaphthalene O2
C ₉ H ₁₆ ClN ₃ O ₂	lomustine L58	C ₁₀ Cl ₁₀	dienochlor D277
C ₉ H ₁₆ ClN ₃ O ₇	chlorozotocin C307	C ₁₀ Cl ₁₀ O	chlordecone C119
C ₉ H ₁₆ ClN ₅	propazine P302	C ₁₀ Cl ₁₂	mirex M334
C ₉ H ₁₆ ClN ₅	trietazine T275	C ₁₀ HCl ₁₁	photomirex P169
C ₉ H ₁₆ ClN ₅	terbutylazine T24	C ₁₀ H ₂ Cl ₆	hexachloronaphthalene H39
C ₉ H ₁₆ Cl ₂ N ₄	<i>N</i> -(3-chloroallyl)hexaminium chloride C153	C ₁₀ H ₂ N ₂ S ₄ Zn	zinc diethyldithiocarbamate Z9
C ₉ H ₁₆ N ₃ O ₅ P	iproniazid phosphate I63	C ₁₀ H ₂ O ₆	pyromellitic dianhydride P364
C ₉ H ₁₆ N ₄ OS	tebuthiuron T13	C ₁₀ H ₃ Cl ₅	pentachloronaphthalene P29
C ₉ H ₁₆ O ₂	hexyl acrylate H78	C ₁₀ H ₄ Cl ₂ FNO ₂	fluoromide F67
C ₉ H ₁₆ O ₂	4-hydroxy-2-nonenal H114	C ₁₀ H ₄ Cl ₂ O ₂	dichlone D169
C ₉ H ₁₇ ClN ₃ O ₃ PS	isazofos I79	C ₁₀ H ₅ ClN ₂	2-chlorobenzylidenemalononitrile C175
C ₉ H ₁₇ ClO ₂	2-ethylhexyl chloroformate E133	C ₁₀ H ₅ Cl ₇	heptachlor H15
C ₉ H ₁₇ N	octyl cyanide O21	C ₁₀ H ₅ Cl ₇ O	heptachlor epoxide H16
		C ₁₀ H ₅ Cl ₉	<i>trans</i> -nonachlor N190
		C ₁₀ H ₆ ClNO ₂	quinoclamine Q8
		C ₁₀ H ₆ Cl ₄ O ₄	chlorthal-dimethyl C317

$C_{10}H_6Cl_8$	chlordane C118	$C_{10}H_{10}Cl_2O_2$	chlorfenprop-methyl C126
$C_{10}H_6F_{17}NO_2S$	sulfuramid S142	$C_{10}H_{10}Cl_2O_3$	2,4-DB D25
$C_{10}H_6N_2OS_2$	quinomethionate Q11	$C_{10}H_{10}Cl_2Ti$	titanocene dichloride T168
$C_{10}H_6N_2O_4$	dinitronaphthalene D480	$C_{10}H_{10}Cl_3O_4P$	dimethylvinphos D460
$C_{10}H_6N_2O_4$	1,3-dinitronaphthalene D481	$C_{10}H_{10}Cl_8$	camphechlor C48
$C_{10}H_6N_2O_4$	1,8-dinitronaphthalene D483	$C_{10}H_{10}Fe$	ferrocene F32
$C_{10}H_6N_2O_4$	1,5-dinitronaphthalene D482	$C_{10}H_{10}N_2$	1,5-naphthalenediamine N10
$C_{10}H_6O_2$	1,4-naphthoquinone N20	$C_{10}H_{10}N_2O$	1-phenyl-3-methyl-5-pyrazolone P121
$C_{10}H_7Cl$	2-chloronaphthalene C218		metamitron M95
$C_{10}H_7Cl$	1-chloronaphthalene C217	$C_{10}H_{10}N_4O$	sulfadiazine S132
$C_{10}H_7Cl_5O_2$	plifenate P215	$C_{10}H_{10}N_4O_2S$	tetralone T82
$C_{10}H_7NO_2$	1-nitroso-2-naphthol N167	$C_{10}H_{10}O$	α -tetralone T83
$C_{10}H_7NO_2$	2-nitroso-1-naphthol N168	$C_{10}H_{10}O$	β -tetralone T84
$C_{10}H_7NO_2$	1-nitronaphthalene N128	$C_{10}H_{10}O$	isosafole I136
$C_{10}H_7NO_2$	2-nitronaphthalene N129	$C_{10}H_{10}O_2$	cinnamyl formate C348
$C_{10}H_7N_3S$	thiabendazole T111	$C_{10}H_{10}O_2$	safrole S2
$C_{10}H_8$	naphthalene N9	$C_{10}H_{10}O_2$	dimethyl terephthalate D459
$C_{10}H_8ClN_3O$	chloridazon C131	$C_{10}H_{10}O_4$	dimethyl phthalate D450
$C_{10}H_8ClN_3O_2$	drazoxolon D600	$C_{10}H_{10}O_4$	mecoprop M40
$C_{10}H_8N_2$	indole-3-acetonitrile I33	$C_{10}H_{11}ClO_3$	fluometuron F47
$C_{10}H_8N_2O_2S_2Zn$	zinc pyrrhione Z15	$C_{10}H_{11}F_3N_2O$	tryptophol T370
$C_{10}H_8N_4$	Glu-P-2 G20	$C_{10}H_{11}NO$	methabenzthiazuron M101
$C_{10}H_8O$	1-naphthol N17	$C_{10}H_{11}N_3OS$	sulfamethoxazole S136
$C_{10}H_8O$	2-naphthol N18	$C_{10}H_{11}N_3O_3S$	dicyclopentadiene D271
$C_{10}H_8O_3$	7-methoxycoumarin M133	$C_{10}H_{12}$	5-methylindan M237
$C_{10}H_9Cl_4NO_2S$	captafol C58	$C_{10}H_{12}$	3-ethylstyrene E170
$C_{10}H_9Cl_4O_4P$	tetrachlorvinphos T60	$C_{10}H_{12}$	4-ethylstyrene E171
$C_{10}H_9N$	8-methylquinoline M303	$C_{10}H_{12}$	tetralin T80
$C_{10}H_9N$	1-naphthylamine N23	$C_{10}H_{12}$	bromophos-ethyl B184
$C_{10}H_9N$	7-methylquinoline M302	$C_{10}H_{12}BrCl_2O_3PS$	EDTA calcium disodium salt E4
$C_{10}H_9N$	6-methylquinoline M301	$C_{10}H_{12}CaN_2Na_2O_8$	chlorpropham C312
$C_{10}H_9N$	4-methylquinoline M299	$C_{10}H_{12}ClNO_2$	carbanolate C62
$C_{10}H_9N$	5-methylquinoline M300	$C_{10}H_{12}ClNO_2$	bis-1,4-(chloromethoxy)- <i>p</i> -xylene B122
$C_{10}H_9N$	2-naphthylamine N24	$C_{10}H_{12}Cl_2O_2$	trichloronate T253
$C_{10}H_9N$	quinaldine Q4		tryptamine T367
$C_{10}H_9NO_2$	indole-3-acetic acid I32	$C_{10}H_{12}Cl_3O_2PS$	bentazone B38
$C_{10}H_9NO_3S$	7-aminonaphthalene-2-sulfonic acid A135	$C_{10}H_{12}N_2$	3-nitro- <i>p</i> -acetophenelide N72
$C_{10}H_9NO_3S$	8-aminonaphthalene-2-sulfonic acid A136	$C_{10}H_{12}N_2O_3S$	dinoseb D510
$C_{10}H_9NO_3S$	4-aminonaphthalene-1-sulfonic acid A132	$C_{10}H_{12}N_2O_4$	dinoterb D512
$C_{10}H_9NO_3S$	6-aminonaphthalene-2-sulfonic acid A134	$C_{10}H_{12}N_2O_5$	EDTA zinc salt E10
$C_{10}H_9NO_3S$	2-aminonaphthalene-1-sulfonic acid A131	$C_{10}H_{12}N_2O_5$	azinphos-methyl A264
$C_{10}H_9NO_3S$	5-aminonaphthalene-2-sulfonic acid A133	$C_{10}H_{12}N_2O_8Zn$	didanosine D273
$C_{10}H_9N_5O$	kinetin K11	$C_{10}H_{12}N_3O_3PS_2$	inosine I36
$C_{10}H_{10}$	divinylbenzene D580	$C_{10}H_{12}N_4O_3$	EDTA tetrasodium salt E8
$C_{10}H_{10}ClNO_2$	4-(chloroacetyl)acetanilide C150	$C_{10}H_{12}N_4O_5$	4-allylanisole A75
$C_{10}H_{10}Cl_2Hf$	hafnocene dichloride H3	$C_{10}H_{12}Na_4N_2O_8$	4-isopropylbenzaldehyde I122
		$C_{10}H_{12}O$	4-cresyl glycidyl ether C462
		$C_{10}H_{12}O$	isoeugenol I102
		$C_{10}H_{12}O_2$	2-cresyl glycidyl ether C461
		$C_{10}H_{12}O_2$	cresyl glycidyl ether C460

$C_{10}H_{12}O_2$	eugenol E187	$C_{10}H_{14}O$	D-carvone C93
$C_{10}H_{12}O_2$	dihydrosafrole D347	$C_{10}H_{14}O_2$	<i>tert</i> -butylhydroquinone B262
$C_{10}H_{12}O_2$	phenethyl acetate P66	$C_{10}H_{14}O_4$	guaiphenesin G47
$C_{10}H_{12}O_2$	tetralin hydroperoxide T81	$C_{10}H_{14}O_4$	1,4-butanediol diacrylate B207
$C_{10}H_{12}O_3$	propylparaben P336	$C_{10}H_{14}O_4$	ethylene glycol dimethacrylate E119
$C_{10}H_{12}O_4$	cantharidin C54		
$C_{10}H_{12}O_5$	propyl gallate P332	$C_{10}H_{14}O_4$	1,3-butanediol diacrylate B206
$C_{10}H_{12}S_2$	2-phenyl-1,3-dithiane P99	$C_{10}H_{14}O_5$	diethylene glycol diacrylate D302
$C_{10}H_{13}ClN_2$	chlordimeform C121	$C_{10}H_{15}N$	<i>N</i> -butylaniline B242
$C_{10}H_{13}ClN_2O$	chlorotoluron C298	$C_{10}H_{15}N$	phentermine P88
$C_{10}H_{13}ClN_2O_2$	metoxuron M325	$C_{10}H_{15}N$	<i>N,N</i> -diethylaniline D291
$C_{10}H_{13}ClN_2O_3S$	chlorpropamide C311	$C_{10}H_{15}NO$	ephedrine E30
$C_{10}H_{13}Cl_2FN_2O_2S_2$	tolyfluanid T191	$C_{10}H_{15}NO_2S$	<i>N</i> -butylbenzenesulfonamide B248
$C_{10}H_{13}Cl_2NO_3$	2,4-D, dimethylamine salt D8	$C_{10}H_{15}N_5$	phenformin P74
$C_{10}H_{13}Cl_2O_3PS$	dichlofenthion D167	$C_{10}H_{15}OPS_2$	fonofos F99
$C_{10}H_{13}Cl_4N_3Zn$	3-chloro-4-diethylaminobenzene-diazonium trichlorozincate C190	$C_{10}H_{15}O_2PS_2$	<i>O</i> -ethyl <i>O</i> -[4-(methylthio)phenyl] methylphosphonothioate E150
			fenthion F24
$C_{10}H_{13}NO_2$	propham P305	$C_{10}H_{15}O_3PS_2$	camphene C49
$C_{10}H_{13}NO_2$	phenacetin P58	$C_{10}H_{16}$	limonene L45
$C_{10}H_{13}NO_2$	XMC X4	$C_{10}H_{16}$	myrcene M361
$C_{10}H_{13}NO_2$	xylylcarb X16	$C_{10}H_{16}$	α -pinene P195
$C_{10}H_{13}NO_4$	methyl dopa M208	$C_{10}H_{16}$	β -pinene P198
$C_{10}H_{13}N_3$	debrisoquine D36	$C_{10}H_{16}$	terpinolene T37
$C_{10}H_{13}N_3O_2$	NNK N189	$C_{10}H_{16}$	(\pm)- α -pinene P197
$C_{10}H_{13}N_3O_3$	<i>N</i> -(2-methyl-2-nitropropyl)-4-nitrosoaniline M266	$C_{10}H_{16}$	α -terpinene T34
		$C_{10}H_{16}$	(<i>R</i>)-(+)-limonene L46
$C_{10}H_{13}Na_3N_2O_8$	EDTA trisodium salt E9	$C_{10}H_{16}$	(1 <i>R</i>)-(+)- α -pinene P196
$C_{10}H_{14}$	butylbenzene B246	$C_{10}H_{16}$	(1 <i>S</i>)-(-)- β -pinene P199
$C_{10}H_{14}$	<i>tert</i> -butylbenzene B247	$C_{10}H_{16}$	adamantane A47
$C_{10}H_{14}$	1,4-diethylbenzene D294	$C_{10}H_{16}$	(1 <i>S</i>)-(-)- α -pinene P194
$C_{10}H_{14}$	<i>o</i> -cymene C539	$C_{10}H_{16}$	tri-allate T198
$C_{10}H_{14}$	cymene C537	$C_{10}H_{16}Cl_3NOS$	famphur F1
$C_{10}H_{14}$	1,2-diethylbenzene D292	$C_{10}H_{16}NO_5PS_2$	<i>N,N</i> -diethyl- <i>p</i> -phenylenediamine D313
$C_{10}H_{14}$	1,3-diethylbenzene D293	$C_{10}H_{16}N_2$	<i>N,N,N',N'</i> -tetramethyl- <i>p</i> -phenylenediamine T92
$C_{10}H_{14}$	<i>m</i> -cymene C538		butobarbitone B222
$C_{10}H_{14}$	durene D602	$C_{10}H_{16}N_2$	biotin B112
$C_{10}H_{14}$	1,2,3,5-tetramethylbenzene T88		EDTA E3
$C_{10}H_{14}$	1,2,3,4-tetramethylbenzene T87	$C_{10}H_{16}N_2O_3$	dimetilan D462
$C_{10}H_{14}$	<i>p</i> -cymene C540	$C_{10}H_{16}N_2O_3S$	(-)-camphor C52
$C_{10}H_{14}Cl_6N_4O_2$	triforine T295	$C_{10}H_{16}N_2O_8$	(\pm)-camphor C53
$C_{10}H_{14}CuN_2Na_2O_9$	copper EDTA C436	$C_{10}H_{16}N_4O_3$	(+)-camphor C51
$C_{10}H_{14}CuN_2O_8$	EDTA copper complex E5	$C_{10}H_{16}O$	camphor C50
$C_{10}H_{14}K_2N_2O_8$	EDTA dipotassium salt E6	$C_{10}H_{16}O$	isocyclocitral I100
$C_{10}H_{14}NO_5PS$	parathion P13	$C_{10}H_{16}O$	citral C351
$C_{10}H_{14}NO_6P$	paraoxon P10	$C_{10}H_{16}O$	di-allate D69
$C_{10}H_{14}N_2$	nicotine N54	$C_{10}H_{16}O$	etrimfos E186
$C_{10}H_{14}N_2Na_2O_8$	EDTA disodium salt E7	$C_{10}H_{17}Cl_2NOS$	isouron I139
$C_{10}H_{14}N_4O_2$	isobutylmethylxanthine I93	$C_{10}H_{17}N_2O_4PS$	isolan I107
$C_{10}H_{14}O$	myrtenal M365	$C_{10}H_{17}N_3O_2$	<i>trans</i> -decahydronaphthalene D39
$C_{10}H_{14}O$	2- <i>sec</i> -butylphenol B275	$C_{10}H_{17}N_3O_2$	
$C_{10}H_{14}O$	4- <i>tert</i> -butylphenol B276	$C_{10}H_{18}$	
$C_{10}H_{14}O$	thymol T154		

$C_{10}H_{18}$	<i>cis</i> -decahydronaphthalene D38	$C_{10}H_{24}Cl_4N_2O_4$	mannomustine hydrochloride M29
$C_{10}H_{18}N_4O_4S_3$	thiodicarb T128		amiton A156
$C_{10}H_{18}O$	isopulegol I134	$C_{10}H_{24}NO_3PS$	spermine S107
$C_{10}H_{18}O$	cineole C343	$C_{10}H_{26}N_4$	pentaethylenehexamine P38
$C_{10}H_{18}O$	geraniol G12	$C_{10}H_{28}N_6$	psoralen P344
$C_{10}H_{18}O$	borneol B143	$C_{11}H_6O_3$	cytembena C547
$C_{10}H_{18}O$	linalool L47	$C_{11}H_8BrO_4Na$	α -carboline C70
$C_{10}H_{18}O$	α -terpineol T36	$C_{11}H_8N_2$	β -carboline C71
$C_{10}H_{18}O$	terpineol T35	$C_{11}H_8N_2$	γ -carboline C72
$C_{10}H_{18}O_4$	1,4-butanediol diglycidyl ether B208	$C_{11}H_8N_2O$	fuberidazole F113
$C_{10}H_{18}O_4$	diethyl adipate D287	$C_{11}H_8N_2O_5$	furylamide F132
$C_{10}H_{18}O_4$	sebacic acid S11	$C_{11}H_8O$	1-naphthaldehyde N7
$C_{10}H_{18}O_6$	dibutyl peroxydicarbonate D152	$C_{11}H_8O$	2-naphthaldehyde N8
	di- <i>sec</i> -butyl peroxydicarbonate D153	$C_{11}H_8O_2$	2-naphthoic acid N16
$C_{10}H_{18}O_6$	phosphamidon P154	$C_{11}H_8O_2$	1-naphthoic acid N15
$C_{10}H_{19}ClNO_5P$	cyanthoate C490	$C_{11}H_8O_3$	plumbagin P216
$C_{10}H_{19}N_2O_4PS$	terbumeton T23	$C_{11}H_9Cl_2NO_2$	barban B4
$C_{10}H_{19}N_5O$	prometon P288	$C_{11}H_9Cl_5O_3$	2-(2,4,5-trichlorophenoxy)ethyl 2,2-dichloropropionate T261
$C_{10}H_{19}N_5O$	terbutryn T25		A- α -C A1
$C_{10}H_{19}N_5S$	prometryn P289	$C_{11}H_9N_3$	1-methylnaphthalene M257
$C_{10}H_{19}N_5S$	malathion M11	$C_{11}H_{10}$	methylnaphthalene M256
$C_{10}H_{19}O_6PS_2$	malaoxon M10	$C_{11}H_{10}$	2-methylnaphthalene M258
$C_{10}H_{19}O_7PS$	1,1-dimethylethylcyclohexane D415	$C_{11}H_{10}ClNO_2$	chlorbufam C117
$C_{10}H_{20}$	<i>trans</i> - <i>p</i> -menthane M51	$C_{11}H_{10}N_2S$	1-naphthylthiourea N27
$C_{10}H_{20}$	1,10-dibromodecane D129	$C_{11}H_{10}N_4$	Glu-P-1 G19
$C_{10}H_{20}Br_2$	propetamphos P304	$C_{11}H_{10}O_3$	7-ethoxycoumarin E75
$C_{10}H_{20}NO_4PS$	mecarbam M37	$C_{11}H_{11}NO$	pyroquilon P365
$C_{10}H_{20}NO_5PS_2$	disulfiram D565	$C_{11}H_{11}N_2O_5$	dihydroxymethylfuratrizine D350
$C_{10}H_{20}N_2S_4$	menthol M53	$C_{11}H_{11}N_5$	phenazopyridine P62
$C_{10}H_{20}O$	decanal D40	$C_{11}H_{12}$	2,3-dimethylindene D425
$C_{10}H_{20}O$	DL-menthol M54	$C_{11}H_{12}ClN_5$	phenazopyridine hydrochloride P63
$C_{10}H_{20}O_2$	<i>p</i> -menthane hydroperoxide M52		chloramphenicol C114
$C_{10}H_{20}O_2$	terpin T32	$C_{11}H_{12}Cl_2N_2O_5$	2,4-D, isopropyl ester D11
$C_{10}H_{20}O_2$	<i>cis</i> -1,8-terpin T33	$C_{11}H_{12}Cl_2O_3$	monuron-TCA M351
$C_{10}H_{20}O_2S$	2-ethylhexyl mercaptoacetate E134	$C_{11}H_{12}Cl_4N_2O_3$	phosmet P153
	2-(2-butoxyethoxy)ethanol acetate B228	$C_{11}H_{12}NO_4PS_2$	L-tryptophan T369
$C_{10}H_{20}O_4$	vernolate V19	$C_{11}H_{12}N_2O_2$	D-tryptophan T368
$C_{10}H_{21}NOS$	pebulate P17	$C_{11}H_{12}N_2O_2$	allyl phenylacetate A91
$C_{10}H_{21}NOS$	decane D41	$C_{11}H_{12}O_2$	allyl phenoxyacetate A90
$C_{10}H_{22}$	isophorone diamine I111	$C_{11}H_{12}O_3$	4-chloro-2-cyclopentylphenol C189
$C_{10}H_{22}N_2$	1-decanol D42	$C_{11}H_{13}ClO$	MCPA-thioethyl M33
$C_{10}H_{22}O$	pentyl ether P48		MCPB M34
$C_{10}H_{22}O$	1,2-dibutoxyethane D138	$C_{11}H_{13}ClO_2S$	mefluidide M43
$C_{10}H_{22}O_2$	dipentylamine D533	$C_{11}H_{13}F_3N_2O_3S$	dinitramine D466
$C_{10}H_{23}N$	2-dibutylaminoethanol D143	$C_{11}H_{13}F_3N_4O_4$	decarbofuran D43
$C_{10}H_{23}NO$	cadusafos C15	$C_{11}H_{13}NO_3$	bendiocarb B28
$C_{10}H_{23}O_2PS_2$		$C_{11}H_{13}NO_4$	dioxacarb D528
		$C_{11}H_{13}NO_4$	4-aminoantipyrine A113
		$C_{11}H_{13}N_3O$	

C ₁₁ H ₁₃ N ₃ O ₃ S	sulfisoxazole S141	C ₁₁ H ₂₂ N ₃ O ₆ P	bilanafos B110
C ₁₁ H ₁₄ ClNO	propachlor P290	C ₁₁ H ₂₂ O	undecanal U1
C ₁₁ H ₁₄ ClNO ₄	cloethocarb C356	C ₁₁ H ₂₂ O	6-undecanone U7
C ₁₁ H ₁₄ N ₂	gramine G44	C ₁₁ H ₂₂ O	2-undecanone U6
C ₁₁ H ₁₄ N ₂ O ₄	nitrosopropoxur N173	C ₁₁ H ₂₂ O ₂	undecanoic acid U4
C ₁₁ H ₁₄ N ₂ O ₅	dinosam D509	C ₁₁ H ₂₃ ClOS	3-chloropropyl octyl sulfoxide C277
C ₁₁ H ₁₄ O ₂	4- <i>tert</i> -butylbenzoic acid B249		butylate B243
C ₁₁ H ₁₄ O ₂	methyleugenol M223	C ₁₁ H ₂₃ NOS	11-aminoundecanoic acid A155
C ₁₁ H ₁₄ O ₃	<i>tert</i> -butyl peroxybenzoate B271	C ₁₁ H ₂₃ NO ₂	undecane U2
C ₁₁ H ₁₄ O ₃	butylparaben B269	C ₁₁ H ₂₄	1-undecanol U5
C ₁₁ H ₁₅ BrClO ₃ PS	profenofos P279	C ₁₁ H ₂₄ O	1-undecanethiol U3
C ₁₁ H ₁₅ Cl ₂ O ₂ PS ₂	prothiofos P341	C ₁₁ H ₂₄ S	etacelasil E54
C ₁₁ H ₁₅ Cl ₂ O ₂ PS ₃	phenkapton P77	C ₁₁ H ₂₅ ClO ₆ Si	VX V41
C ₁₁ H ₁₅ Cl ₂ O ₃ PS ₂	chlorthiophos C321	C ₁₁ H ₂₆ NO ₂ PS	pentabromophenyl ether P24
C ₁₁ H ₁₅ NO ₂	isoprocarb I116	C ₁₂ Br ₁₀ O	perfluorotributylamine P55
C ₁₁ H ₁₅ NO ₂	2,3,4-trimethacarb T300	C ₁₂ F ₂₇ N	1,2,3,7,8,9-hexachlorodibenzo- <i>p</i> -dioxin H37
C ₁₁ H ₁₅ NO ₂	3,4,5-trimethacarb T301	C ₁₂ H ₂ Cl ₆ O ₂	1,2,3,6,7,8-hexachlorodibenzo- <i>p</i> -dioxin H36
C ₁₁ H ₁₅ NO ₂	3-isopropylphenyl methylcarbamate I131		polybrominated biphenyls P219
C ₁₁ H ₁₅ NO ₂ S	ethiofencarb E67	C ₁₂ H ₄ Br ₆	2,2',4,4',5,5'-hexabromobiphenyl H31
C ₁₁ H ₁₅ NO ₂ S	methiocarb M123	C ₁₂ H ₄ Br ₆	fipronil F33
C ₁₁ H ₁₅ NO ₃	propoxur P315		4,5-dichloronaphthalene-1,8-dicarboxylic anhydride D226
C ₁₁ H ₁₅ NO ₅	methocarbamol M125	C ₁₂ H ₄ Cl ₂ F ₆ N ₄ OS	sodium bithionolate S49
C ₁₁ H ₁₅ N ₃ O ₂	formetate F102	C ₁₂ H ₄ Cl ₂ O ₃	dibenzo- <i>p</i> -dioxin, 2,3,7,8-tetrachloro- D110
C ₁₁ H ₁₆	4- <i>tert</i> -butyltoluene B278	C ₁₂ H ₄ Cl ₂ O ₃	Aroclor 1254 A238
C ₁₁ H ₁₆ ClN ₃ O ₂	formetate hydrochloride F103		1,2,3,4-tetranitrocarbazole T94
C ₁₁ H ₁₆ ClO ₂ PS ₃	carbophenothion C82	C ₁₂ H ₄ Cl ₄ Na ₂ O ₂ S	dipicrylamine D550
C ₁₁ H ₁₆ N ₂ O ₂	aminocarb A123	C ₁₂ H ₄ Cl ₄ O ₂	dibenzo- <i>p</i> -dioxin, 1,6-dichloro- D109
C ₁₁ H ₁₆ N ₂ O ₂	pilocarpine P189		dibenzo- <i>p</i> -dioxin, 2,7-dichloro- D105
C ₁₁ H ₁₆ O	jasmone J3	C ₁₂ H ₅ Cl ₅	2,2'-thiobis(4,6-dichlorophenol) T122
C ₁₁ H ₁₆ O	4- <i>tert</i> -amylphenol A205	C ₁₂ H ₅ N ₅ O ₈	tetradifon T63
C ₁₁ H ₁₆ O ₂	butylated hydroxyanisole B244	C ₁₂ H ₅ N ₇ O ₁₂	tetrasul T98
C ₁₁ H ₁₆ O ₂	dihydroactinidolide D342	C ₁₂ H ₆ Cl ₂ O ₂	naphthalene 1,5-diisocyanate N11
C ₁₁ H ₁₆ O ₄	neopentyl glycol diacrylate N41		dibenzofuran, chlorinated D112
C ₁₁ H ₁₇ ClN ₂ O ₂	pilocarpine hydrochloride P190	C ₁₂ H ₆ Cl ₂ O ₂	dibenzo- <i>p</i> -dioxin, 2-chloro- D108
C ₁₁ H ₁₇ NO ₃	orciprenaline O33		dibenzo- <i>p</i> -dioxin, 1-chloro- D107
C ₁₁ H ₁₇ NO ₃	dimetan D370	C ₁₂ H ₆ Cl ₄ O ₂ S	nitrofen N112
C ₁₁ H ₁₇ O ₄ PS ₂	fensulfothion F23		acenaphthylene A4
C ₁₁ H ₁₈ N ₂ O ₃	pentobarbitone P45	C ₁₂ H ₆ Cl ₄ O ₂ S	4,4'-dibromobiphenyl D125
C ₁₁ H ₁₈ N ₂ O ₃	amylobarbitone A204	C ₁₂ H ₆ Cl ₄ S	bis(4-bromophenyl) ether B115
C ₁₁ H ₁₈ N ₄ O ₂	pirimicarb P208	C ₁₂ H ₆ N ₂ O ₂	2,2'-thiobis(4-chlorophenol) T121
C ₁₁ H ₁₉ NOS	octhlinone O19	C ₁₂ H ₇ ClO	bis(4-chlorophenyl) sulfone B127
C ₁₁ H ₁₉ N ₃ O	ethirimol E70	C ₁₂ H ₇ ClO ₂	chlorfenson C127
C ₁₁ H ₁₉ N ₃ O	dimethirimol D375	C ₁₂ H ₇ ClO ₂	isodrin I101
C ₁₁ H ₂₀ N ₃ O ₃ PS	pirimiphos-methyl P210	C ₁₂ H ₇ Cl ₂ NO ₃	
C ₁₁ H ₂₀ O	2-methylisoborneol M240	C ₁₂ H ₈	
C ₁₁ H ₂₀ O ₂	2-ethylhexyl acrylate E131	C ₁₂ H ₈ Br ₂	
C ₁₁ H ₂₀ O ₂	allyl octanoate A89	C ₁₂ H ₈ Br ₂ O	
C ₁₁ H ₂₁ NOS	cycloate C498	C ₁₂ H ₈ Cl ₂ O ₂ S	
C ₁₁ H ₂₁ N ₅ S	dimethametryn D372	C ₁₂ H ₈ Cl ₂ O ₂ S	
C ₁₁ H ₂₁ N ₅ S	dipropetryn D551	C ₁₂ H ₈ Cl ₂ O ₃ S	
C ₁₁ H ₂₂ N ₂ O	cycluron C532	C ₁₂ H ₈ Cl ₆	

$C_{12}H_8Cl_6$	aldrin A65	$C_{12}H_{11}ClN_2O_5S$	frusemide F112
$C_{12}H_8Cl_6O$	dieldrin D276	$C_{12}H_{11}Cl_2NO$	propyzamide P339
$C_{12}H_8Cl_6O$	endrin E25	$C_{12}H_{11}Cl_2N_3O_2$	azaconazole A256
$C_{12}H_8Cl_6O$	endrin aldehyde E26	$C_{12}H_{11}Cl_3O_3$	2,4-D, 4-chloro-2-butenyl ester D6
$C_{12}H_8Cl_6O$	photodieldrin P168	$C_{12}H_{11}Hg_2NO_4$	phenylmercuric nitrate, basic P120
$C_{12}H_8N_2$	phenazine P61		
$C_{12}H_8N_2$	1,10-phenanthroline P60	$C_{12}H_{11}N$	4-aminobiphenyl A121
$C_{12}H_8O$	dibenzofuran D111	$C_{12}H_{11}N$	2-aminobiphenyl A119
$C_{12}H_8O_2$	dibenzo- <i>p</i> -dioxin D106	$C_{12}H_{11}N$	3-aminobiphenyl A120
$C_{12}H_8O_4$	methoxsalen M129	$C_{12}H_{11}N$	diphenylamine D540
$C_{12}H_9AsClN$	diphenylamine chloroarsine D541	$C_{12}H_{11}NO$	1-naphthylacetamide N21
$C_{12}H_9BrO$	4-bromodiphenyl ether B174	$C_{12}H_{11}NO_2$	carbaryl C63
$C_{12}H_9ClF_3N_3O$	norflurazon N206	$C_{12}H_{11}NO_2$	fenfuram F10
$C_{12}H_9ClN_2O_3$	aclonifen A32	$C_{12}H_{11}N_3$	Trp-P-2 T365
$C_{12}H_9ClO$	2-chloro-4-phenylphenol C249	$C_{12}H_{11}N_3$	4-aminoazobenzene A114
$C_{12}H_9ClO$	4-chlorophenyl phenyl ether C250	$C_{12}H_{11}N_5$	MeIQx M46
$C_{12}H_9ClSO_3$	fenson F22	$C_{12}H_{11}N_7$	triamterene T203
$C_{12}H_9Cl_2NO_3$	vinclozolin V23	$C_{12}H_{12}$	1,8-dimethylnaphthalene D439
$C_{12}H_9NO$	3-dibenzofuranamine D114	$C_{12}H_{12}$	1,5-dimethylnaphthalene D436
$C_{12}H_9NO_2$	4-nitrobiphenyl N100	$C_{12}H_{12}$	1,6-dimethylnaphthalene D437
$C_{12}H_9NO_2$	2-nitrobiphenyl N98	$C_{12}H_{12}$	1,4-dimethylnaphthalene D435
$C_{12}H_9NO_2$	3-nitrobiphenyl N99	$C_{12}H_{12}$	1-ethylnaphthalene E153
$C_{12}H_9NO_2$	5-nitroacenaphthene N71	$C_{12}H_{12}$	1,2-dimethylnaphthalene D433
$C_{12}H_9NS$	phenothiazine P83	$C_{12}H_{12}$	1,7-dimethylnaphthalene D438
$C_{12}H_9NaO$	sodium <i>o</i> -phenylphenolate S86	$C_{12}H_{12}$	2-ethylnaphthalene E154
$C_{12}H_{10}$	biphenyl B113	$C_{12}H_{12}$	2,3-dimethylnaphthalene D440
$C_{12}H_{10}$	acenaphthene A3	$C_{12}H_{12}$	2,7-dimethylnaphthalene D442
$C_{12}H_{10}Cl_2F_3NO$	flurochloridone F87	$C_{12}H_{12}$	2,6-dimethylnaphthalene D441
$C_{12}H_{10}Cl_2N_2$	2,2-dichlorohydrazobenzene D218	$C_{12}H_{12}$	1,3-dimethylnaphthalene D434
$C_{12}H_{10}Cl_2N_2$	2,2'-dichlorobenzidine D191	$C_{12}H_{12}Br_2N_2$	diquat dibromide D561
$C_{12}H_{10}Cl_2N_2$	3,3'-dichlorobenzidine D192	$C_{12}H_{12}ClN_5O_4S$	chlorsulfuron C315
$C_{12}H_{10}Cl_2N_2O$	4,4'-oxybis(2-chloroaniline) O54	$C_{12}H_{12}Cl_4N_2$	3,3'-dichlorobenzidine dihydrochloride D193
$C_{12}H_{10}Cl_2Si$	dichlorodiphenylsilane D209		benzidine B52
$C_{12}H_{10}FN$	4'-fluoro-4-aminobiphenyl F57	$C_{12}H_{12}N_2$	diquat D560
$C_{12}H_{10}N_2$	harmane H6	$C_{12}H_{12}N_2$	1,2-diphenylhydrazine D546
$C_{12}H_{10}N_2$	azobenzene A268	$C_{12}H_{12}N_2$	2,4'-diphenyldiamine D543
$C_{12}H_{10}N_2O$	azoxybenzene A274	$C_{12}H_{12}N_2$	<i>N</i> -phenyl- <i>p</i> -phenylenediamine P128
$C_{12}H_{10}N_2O$	4-nitrosodiphenylamine N154	$C_{12}H_{12}N_2$	4,4'-oxydianiline O58
$C_{12}H_{10}N_2O$	<i>N</i> -nitrosodiphenylamine N155	$C_{12}H_{12}N_2O$	4,4'-sulfonyldianiline S146
$C_{12}H_{10}N_2O$	C.I. Solvent Yellow 7 C425	$C_{12}H_{12}N_2O_2S$	nalidixic acid N4
$C_{12}H_{10}N_2O$	diphenyl ether D544	$C_{12}H_{12}N_2O_3$	oxabetrinil O42
$C_{12}H_{10}O$	2-phenylphenol P125	$C_{12}H_{12}N_2O_3$	phenobarbitone P79
$C_{12}H_{10}O$	3-phenylphenol P126	$C_{12}H_{12}N_2O_3$	4,4'-thiodianiline T127
$C_{12}H_{10}O$	4-phenylphenol P127	$C_{12}H_{12}N_2S$	2,4-diaminoazobenzene D79
$C_{12}H_{10}OS$	phenyl sulfoxide P135	$C_{12}H_{12}N_4$	MeIQ M45
$C_{12}H_{10}O_2$	1-naphthylacetic acid N22	$C_{12}H_{12}N_4$	allyl cinnamate A80
$C_{12}H_{10}O_2$	phenylhydroquinone P110	$C_{12}H_{12}O_2$	chrysoidin C341
$C_{12}H_{10}O_2$	4-phenoxyphenol P87	$C_{12}H_{13}ClN_4$	butyl 2,4,5-trichlorophenoxyacetate B279
$C_{12}H_{10}O_2S$	phenyl sulfone P134	$C_{12}H_{13}Cl_3O_3$	indole-3-butyric acid I34
$C_{12}H_{10}O_3$	(2-naphthylxy)acetic acid N26	$C_{12}H_{13}NO_2$	
$C_{12}H_{10}O_8S_2Zn$	zinc <i>p</i> -phenolsulfonate Z13		
$C_{12}H_{11}ClF_3NO_3$	fluxofenim F95		

$C_{12}H_{13}NO_2S$	carboxin C84	$C_{12}H_{17}NO_3Si$	phenylsilatrane P133
$C_{12}H_{13}NO_4S$	oxycarboxin O56	$C_{12}H_{17}N_3O_2$	formparanate F106
$C_{12}H_{13}N_3O_2$	2,3,5-tris(1-aziridinyl)- <i>p</i> -benzoquinone T345	$C_{12}H_{17}N_3O_4$	agaritine A59
$C_{12}H_{14}ClNO_2$	clomazone C359	$C_{12}H_{17}N_4OSCl$	thiamine T112
$C_{12}H_{14}Cl_2O_3$	2,4-D, butyl ester D4	$C_{12}H_{17}NaO_7$	dikegulac-sodium D362
$C_{12}H_{14}Cl_2O_3$	2,4-D, <i>sec</i> -butyl ester D5	$C_{12}H_{17}O_4PS_2$	phenthoate P89
$C_{12}H_{14}Cl_2O_3$	2,4-D, isobutyl ester D9	$C_{12}H_{18}$	(<i>E,E,Z</i>)-1,5,9-cyclododecatiene C504
$C_{12}H_{14}Cl_3O_4P$	chlorfenvinphos C128	$C_{12}H_{18}$	(<i>E,E,E</i>)-1,5,9-cyclododecatiene C503
$C_{12}H_{14}N_2$	paraquat P11	$C_{12}H_{18}$	1-phenylhexane P107
$(C_{12}H_{14}N_2O)_n$	<i>N</i> -nitroso-2,2,4-trimethyl-1,2-dihydroquinoline, polymers N176	$C_{12}H_{18}N_2O$	isoproturon I133
$C_{12}H_{14}N_2O_2$	primidone P272	$C_{12}H_{18}N_2O$	oxotremorin O51
$C_{12}H_{14}N_2O_5$	2-cyclohexyl-4,6-dinitrophenol C516	$C_{12}H_{18}N_2O_2$	mexacarbate M331
$C_{12}H_{14}N_2O_6$	dinoseb acetate D511	$C_{12}H_{18}N_2O_2$	isophorone diisocyanate I112
$C_{12}H_{14}N_4O_2S$	sulfadimidine S133	$C_{12}H_{18}N_2O_3$	quinalbarbitone Q3
$C_{12}H_{14}N_4O_4S_2$	thiophanate-methyl T138	$C_{12}H_{18}N_2O_3S$	tolbutamide T171
$C_{12}H_{14}N_4O_5S_2$	4,4'-oxybis(benzenesulfonylhydrazide) O53	$C_{12}H_{18}N_4OSCl_2$	thiamine hydrochloride T113
$C_{12}H_{14}N_4PS$	ditalimfos D569	$C_{12}H_{18}N_4O_6S$	oryzalin O36
$C_{12}H_{14}O_2$	cinnamyl propionate C349	$C_{12}H_{18}O$	2,4-dimethyl-6- <i>tert</i> -butylphenol D405
$C_{12}H_{14}O_4$	monobutyl phthalate M341	$C_{12}H_{18}O$	propofol P314
$C_{12}H_{14}O_4$	diethyl phthalate D314	$C_{12}H_{18}O_2$	amyl- <i>m</i> -cresol A199
$C_{12}H_{14}O_4$	resorcinol diglycidyl ether R6	$C_{12}H_{18}O_2$	2- <i>tert</i> -butyl-1,4-dimethoxybenzene B256
$C_{12}H_{14}O_4$	dill apiole D366	$C_{12}H_{18}O_4$	1,6-hexanediol diacrylate H61
$C_{12}H_{14}O_4$	apiole A230	$C_{12}H_{18}O_4S_2$	isoprothiolane I132
$C_{12}H_{15}ClNO_4PS_2$	phosalone P149	$C_{12}H_{18}O_6$	triethylene glycol diacrylate T281
$C_{12}H_{15}ClO_3$	clofibrate C358	$C_{12}H_{19}ClNO_3P$	crufomate C471
$C_{12}H_{15}N$	acetonanil A16	$C_{12}H_{19}NO_4$	choline salicylate C327
$C_{12}H_{15}NO_2$	<i>N,N</i> -diglycidylaniline D336	$C_{12}H_{19}N_3O$	procarbazine P274
$C_{12}H_{15}NO_3$	carbofuran C68	$C_{12}H_{19}N_3O_5$	HC Blue No. 2 H8
$C_{12}H_{15}N_2O_3PS$	phoxim P170	$C_{12}H_{19}N_6OP$	triamphos T202
$C_{12}H_{15}N_2O_3PS$	quinalphos Q5	$C_{12}H_{19}O_2PS_3$	sulprofos S159
$C_{12}H_{15}N_3O_3$	triallyl isocyanurate T201	$C_{12}H_{20}ClN_3O$	ibenzmethylzin hydrochloride I1
$C_{12}H_{15}N_3O_6$	musk xylene M358	$C_{12}H_{20}N_4O_2$	hexazinone H69
$C_{12}H_{16}ClNOS$	thiobencarb T117	$C_{12}H_{20}O_2$	isobornyl acetate I83
$C_{12}H_{16}Cl_2N_2O$	neburon N32	$C_{12}H_{20}O_2$	allyl cyclohexylpropionate A81
$C_{12}H_{16}F_3N$	fenfluramine F9	$C_{12}H_{20}O_7$	triethyl citrate T279
$C_{12}H_{16}N_2Cl_2$	<i>N</i> -(1-naphthyl)ethylenediamine dihydrochloride N25	$C_{12}H_{21}N_2O_3PS$	diazinon D99
$C_{12}H_{16}N_2O_3$	carbetamide C66	$C_{12}H_{22}O$	geosmin G11
$C_{12}H_{16}N_2O_3$	hexobarbital H76	$C_{12}H_{22}O_4$	dipropyl adipate D553
$C_{12}H_{16}N_2O_5$	musk ambrette (synthetic) M357	$C_{12}H_{22}O_4$	diisopropyl adipate D357
$C_{12}H_{16}N_3O_3PS$	triazophos T205	$C_{12}H_{22}O_5$	cyclohexanone hydroperoxide C510
$C_{12}H_{16}N_3O_3PS_2$	azinphos-ethyl A263	$C_{12}H_{22}O_6$	triethylene glycol diglycidyl ether T282
$C_{12}H_{17}Cl_2NO_3$	2,4-D, diethylamine salt D7	$C_{12}H_{22}O_{11}$	β -lactose L3
$C_{12}H_{17}NO$	<i>N,N</i> -diethyl- <i>o</i> -toluamide D320	$C_{12}H_{22}O_{11}$	sucrose S131
$C_{12}H_{17}NO$	<i>N,N</i> -diethyl- <i>m</i> -toluamide D319	$C_{12}H_{23}N$	dicyclohexylamine D265
$C_{12}H_{17}NO$	<i>N,N</i> -diethyl- <i>p</i> -toluamide D321	$C_{12}H_{24}N_2O_2$	dicyclohexylammonium nitrite D266
$C_{12}H_{17}NO_2$	fenobucarb F12		
$C_{12}H_{17}NO_2$	promecarb P286		

$C_{12}H_{24}N_9P_3$	apholate A229	$C_{13}H_{10}O_3$	4-benzoylresorcinol B85
$C_{12}H_{24}O$	dodecanal D584	$C_{13}H_{10}O_3$	phenyl salicylate P132
$C_{12}H_{24}O_2$	lauric acid L8	$C_{13}H_{11}ClO$	2-benzyl-4-chlorophenol B96
$C_{12}H_{24}O_2$	2,2,4-trimethylpentyl isobutyrate T319	$C_{13}H_{11}Cl_2F_4N_3O$	tetraconazole T61
$C_{12}H_{25}NaO_4S$	sodium lauryl sulfate S76	$C_{13}H_{11}Cl_2NO_2$	procymidone P277
$C_{12}H_{26}$	dodecane D585	$C_{13}H_{11}Cl_2NO_5$	chlozolinatone C322
$C_{12}H_{26}N_2O$	<i>N</i> -nitroso- <i>N</i> -methylnundecylamine N162	$C_{13}H_{11}N_3O_2$	benquinol B35
$C_{12}H_{26}N_4O_6$	neomycin A N35	$C_{13}H_{12}$	diphenylmethane D547
$C_{12}H_{26}O$	1-dodecanol D588	$C_{13}H_{12}$	4-methylbiphenyl M170
$C_{12}H_{26}O_4$	2,2-di(<i>tert</i> -butylperoxy)butane D151	$C_{13}H_{12}$	2-methylbiphenyl M169
$C_{12}H_{26}O_6P_2S_4$	dioxathion D531	$C_{13}H_{12}$	methylbiphenyl M168
$C_{12}H_{26}S$	<i>tert</i> -dodecanethiol D587	$C_{13}H_{12}ClN_3$	proflavine hydrochloride P280
$C_{12}H_{26}S$	1-dodecanethiol D586	$C_{13}H_{12}Cl_2N_2$	4,4'-methylenebis(2-chloroaniline) M210
$C_{12}H_{27}FSn$	tributyltin fluoride T215	$C_{13}H_{12}NO_4PS$	<i>O</i> -(4-nitrophenyl) <i>O</i> -phenyl methylphosphonothioate N137
$C_{12}H_{27}N$	tributylamine T210	$C_{13}H_{12}N_2O$	harmine H7
$C_{12}H_{27}OPS_3$	tribufos T209	$C_{13}H_{12}N_2S$	thiocarbanilide T123
$C_{12}H_{27}O_4P$	tributyl phosphate T212	$C_{13}H_{12}N_4$	PhIP P144
$C_{12}H_{27}PS_3$	merphos M89	$C_{13}H_{12}N_4O_3$	pyrinuron P362
$C_{12}H_{28}NO_7PS$	amiton oxalate A157	$C_{13}H_{12}N_4S$	dithizone D576
$C_{12}H_{28}O_4Ti$	tetrapropyl orthotitanate T97	$C_{13}H_{13}Cl_2N_3O_3$	iprodione I62
$C_{12}H_{28}O_5P_2S_2$	tetrapropyl dithiopyrophosphate T96	$C_{13}H_{13}N_3$	1,3-diphenylguanidine D545
$C_{12}H_{30}O_{13}P_4$	hexaethyl tetraphosphate H44	$C_{13}H_{13}N_3$	Trp-P-1 T364
$C_{12}NH_9$	carbazole C64	$C_{13}H_{14}$	2-isopropyl-naphthalene I128
$C_{12}N_{17}N_3O$	azopropcarbazine A272	$C_{13}H_{14}F_3N_3O_4$	ethalfuralin E56
$C_{13}Cl_2H_{16}N_2$	4,4'-methylenedianiline dihydrochloride M219	$C_{13}H_{14}N_2$	4,4'-methylenedianiline M218
$C_{13}H_5N_3O_7$	2,4,7-trinitrofluorenone T330	$C_{13}H_{14}N_2$	2,4'-methylenedianiline M217
$C_{13}H_6Cl_6O_2$	hexachlorophene H41	$C_{13}H_{14}N_2O$	phenylramidol P140
$C_{13}H_7Br_2N_3O_6$	bromofenoxim B176	$C_{13}H_{14}N_4O$	1,5-diphenylcarbazine D542
$C_{13}H_7Cl_2F_3N_2O_4S$	flusulfamide F91	$C_{13}H_{14}O_5$	citrinin C353
$C_{13}H_8Br_3NO_2$	3,4',5'-tribromosalicylanilide T208	$C_{13}H_{15}Cl_2N_3$	penconazole P18
$C_{13}H_8Cl_2N_2O_4$	niclosamide N52	$C_{13}H_{15}NO_2$	glutethimide G22
$C_{13}H_8F_2O_3$	diflunisal D328	$C_{13}H_{15}N_3O_3$	imazapyr I6
$C_{13}H_8O$	9-fluorenone F50	$C_{13}H_{16}F_3N_3O_4$	benfluralin B29
$C_{13}H_8O_2$	xanthone X3	$C_{13}H_{16}F_3N_3O_4$	trifluralin T294
$C_{13}H_9Cl_2NO_4$	chlomethoxyfen C106	$C_{13}H_{16}NO_4PS$	isoxathion I143
$C_{13}H_9Cl_3N_2O$	triclocarban T270	$C_{13}H_{16}N_2O_2$	melatonin M48
$C_{13}H_9N$	acridine A34	$C_{13}H_{16}N_4O_6$	furaltadone F122
$C_{13}H_9NO_2$	2-nitrofluorene N114	$C_{13}H_{16}O_4$	monopentyl phthalate M347
$C_{13}H_{10}$	fluorene F49	$C_{13}H_{17}ClN_4O_6$	oxazolidinone hydrochloride O49
$C_{13}H_{10}BrCl_2O_2PS$	leptophos L35	$C_{13}H_{17}F_3N_4O_4$	prodiamine P278
$C_{13}H_{10}Cl_2O_2$	dichlorophen D235	$C_{13}H_{17}NO$	crotamiton C466
$C_{13}H_{10}INO$	benodanil B31	$C_{13}H_{17}NO_4$	dipropyl 2,5-pyridinedicarboxylate D559
$C_{13}H_{10}N_2$	phenzidole P143	$C_{13}H_{17}N_3O$	aminopyrine A154
$C_{13}H_{10}N_2O_4$	thalidomide T99	$C_{13}H_{18}ClNO$	monalide M340
$C_{13}H_{10}O$	benzophenone B70	$C_{13}H_{18}ClNO_2$	dimethachlor D371
$C_{13}H_{10}O$	xanthene X1	$C_{13}H_{18}Cl_2N_2O_2$	melphalan M49
$C_{13}H_{10}O_2$	phenyl benzoate P94	$C_{13}H_{18}Cl_2N_2O_2$	merphalan M88
		$C_{13}H_{18}N_2O_2$	lenacil L34
		$C_{13}H_{18}O_2$	ibuprofen I2

C ₁₃ H ₁₈ O ₅ S	ethofumesate E72	C ₁₄ H ₉ Cl ₅	<i>p,p'</i> -DDT D35
C ₁₃ H ₁₉ ClNO ₃ PS ₂	anilofofos A212	C ₁₄ H ₉ Cl ₅	<i>o,p'</i> -DDT D34
C ₁₃ H ₁₉ NO	diethylpropion D315	C ₁₄ H ₉ Cl ₅ O	dicofol D261
C ₁₃ H ₁₉ NO ₂ S	fenothiocarb F15	C ₁₄ H ₉ NO ₂	2-aminoanthraquinone A112
C ₁₃ H ₁₉ N ₃ O ₄	pendimethalin P20	C ₁₄ H ₁₀	diphenylacetylene D539
C ₁₃ H ₁₉ N ₃ O ₆ S	nitralin N64	C ₁₄ H ₁₀	anthracene A218
C ₁₃ H ₁₉ O ₅	2,2',4,4'-tetrahydroxybenzophenone T78	C ₁₄ H ₁₀	phenanthrene P59
C ₁₃ H ₂₀ NOCl	diethylpropion hydrochloride D316	C ₁₄ H ₁₀ Cl ₂	<i>p,p'</i> -DDMS D32
C ₁₃ H ₂₀ N ₂ O ₂	procaine P273	C ₁₄ H ₁₀ Cl ₂ O ₂	bis(4-chlorophenyl)acetic acid B125
C ₁₃ H ₂₀ O	α-ionone I57	C ₁₄ H ₁₀ Cl ₄	<i>o,p'</i> -DDD D29
C ₁₃ H ₂₀ O	β-ionone I58	C ₁₄ H ₁₀ Cl ₄	<i>p,p'</i> -DDD D30
C ₁₃ H ₂₁ NO ₃	salbutamol S3	C ₁₄ H ₁₀ N ₂ O ₂	2,6-diaminoanthraquinone D78
C ₁₃ H ₂₁ N ₂ O ₄ PS	butamifos B198	C ₁₄ H ₁₀ N ₂ O ₂	1,2-diaminoanthraquinone D75
C ₁₃ H ₂₁ O ₃ PS	iprobenfos I61	C ₁₄ H ₁₀ N ₂ O ₂	1,4-diaminoanthraquinone D76
C ₁₃ H ₂₁ O ₄ PS	propaphos P298	C ₁₄ H ₁₀ N ₂ O ₂	1,5-diaminoanthraquinone D77
C ₁₃ H ₂₂ NO ₃ PS	fenamiphos F3	C ₁₄ H ₁₀ O ₄	benzoyl peroxide B83
C ₁₃ H ₂₂ N ₂	dicyclohexylcarbodiimide D267	C ₁₄ H ₁₀ O ₄ Hg	mercury benzoate M67
C ₁₃ H ₂₄ N ₂ O	<i>N,N'</i> -dicyclohexylurea D270	C ₁₄ H ₁₁ ClN ₂ O ₄ S	chlorthalidone C318
C ₁₃ H ₂₄ N ₂ S	<i>N,N'</i> -dicyclohexylthiourea D269	C ₁₄ H ₁₁ Cl ₄ O ₄ P	phosdiphen P150
C ₁₃ H ₂₄ N ₃ O ₃ PS	pirimiphos-ethyl P209	C ₁₄ H ₁₁ N	2-aminoanthracene A111
C ₁₃ H ₂₄ N ₄ O ₃ S	bupirimate B193	C ₁₄ H ₁₁ NO ₃	7-ethoxyresorufin E86
C ₁₃ H ₂₆ N ₂	dicykan D272	C ₁₄ H ₁₁ NO ₃	<i>N</i> -phenylphthalamic acid P130
C ₁₃ H ₂₆ O ₃	<i>tert</i> -butyl peroxy-3,5,5-trimethylhexanoate B274	C ₁₄ H ₁₂	stilbene S115
C ₁₃ H ₃₀ N ₃ O ₃ P	cytoxal alcohol cyclohexylammonium salt C548	C ₁₄ H ₁₂ Cl ₂ N ₂ O	pyrifenox P360
C ₁₄ H ₄ N ₂ O ₂ S ₂	dithianon D570	C ₁₄ H ₁₂ Cl ₂ O	2,2-bis(4-chlorophenyl)ethanol B126
C ₁₄ H ₇ Br ₂ NO ₂	1-amino-2,4-dibromoanthraquinone A125	C ₁₄ H ₁₂ Cl ₂ O	chlorfenethol C125
C ₁₄ H ₇ Br ₃ F ₃ N ₃ O ₄	bromethalin B153	C ₁₄ H ₁₂ Cl ₂ O ₂ S	6,6'-thiobis(4-chloro- <i>o</i> -cresol) T120
C ₁₄ H ₇ ClF ₃ NO ₅	acifluorfen A30	C ₁₄ H ₁₂ FNO	<i>N</i> -(4'-fluorobiphen-4-yl)acetamide F62
C ₁₄ H ₇ ClO ₂	2-chloroanthraquinone C160	C ₁₄ H ₁₂ F ₃ NO ₄ S ₂	perfluidone P54
C ₁₄ H ₇ ClO ₂	1-chloroanthraquinone C159	C ₁₄ H ₁₂ N ₂ O ₃ S ₂	2-(4-aminophenyl)-6-methyl-7-benzothiazolesulfonic acid A146
C ₁₄ H ₇ NaO ₅ S	sodium anthraquinone-1-sulfonate S42	C ₁₄ H ₁₂ N ₂ S	2-(4-aminophenyl)-6-methylbenzothiazole A145
C ₁₄ H ₈ Br ₂ F ₃ NO ₂	fluorosalan F72	C ₁₄ H ₁₂ N ₄ O ₂	C.I. Disperse Blue 1 C409
C ₁₄ H ₈ CaI ₂ O ₈	calcium <i>o</i> -iodoxybenzoate C35	C ₁₄ H ₁₂ N ₆ O ₆	nitrovin N184
C ₁₄ H ₈ Cl ₂ N ₄	clofentezine C357	C ₁₄ H ₁₂ O ₂	benzoin B64
C ₁₄ H ₈ Cl ₂ O ₄	4-chlorobenzoyl peroxide C171	C ₁₄ H ₁₂ O ₂	benzyl benzoate B91
C ₁₄ H ₈ Cl ₄	<i>p,p'</i> -DDE D31	C ₁₄ H ₁₃ Cl ₂ N ₂ O ₂ PS	phosacetim P148
C ₁₄ H ₈ N ₂ S ₄	2,2'-dithiobis(benzothiazole) D572	C ₁₄ H ₁₃ N	iminodibenzyl I12
C ₁₄ H ₈ N ₂ S ₄ Zn	zinc 2-mercaptobenzothiazole Z10	C ₁₄ H ₁₃ NO	4-phenylacetanilide P90
C ₁₄ H ₈ O ₂	anthraquinone A220	C ₁₄ H ₁₄ ClNO ₃	cyprofuram C544
C ₁₄ H ₈ O ₄	1,3-dihydroxyanthraquinone D348	C ₁₄ H ₁₄ ClN ₂ O ₃ PS	azothoate A273
C ₁₄ H ₈ O ₄	danthron D22	C ₁₄ H ₁₄ Cl ₂ N ₂ O	imazalil I4
C ₁₄ H ₈ O ₄	quinizarin Q7	C ₁₄ H ₁₄ N ₂	3-amino-9-ethylcarbazole A128
C ₁₄ H ₉ ClF ₂ N ₂ O ₂	diflubenzuron D326	C ₁₄ H ₁₄ N ₂ O	metyrapone M329
C ₁₄ H ₉ Cl ₂ NO ₅	bifenox B108	C ₁₄ H ₁₄ N ₂ O ₆ S ₂	4,4'-diamino-2,2'-stilbenedisulfonic acid D85
C ₁₄ H ₉ Cl ₃	<i>p,p'</i> -DDMU D33	C ₁₄ H ₁₄ N ₃ NaO ₃ S	Methyl Orange M271
		C ₁₄ H ₁₄ O	dibenzyl ether D120

C ₁₄ H ₁₄ O ₂	ethyl 1-naphthylacetate E155	C ₁₄ H ₂₁ NOS	prosulfocarb P340
C ₁₄ H ₁₄ O ₃	naproxen N29	C ₁₄ H ₂₁ NO ₃	furmecyclox F130
C ₁₄ H ₁₄ O ₃	pindone P193	C ₁₄ H ₂₁ NO ₄	diethofencarb D283
C ₁₄ H ₁₄ O ₄	diallyl phthalate D72	C ₁₄ H ₂₁ N ₃ O ₃	karbutilate K4
C ₁₄ H ₁₄ O ₄ NPS	EPN E35	C ₁₄ H ₂₁ N ₃ O ₃ S	tolazamide T170
C ₁₄ H ₁₅ Cl ₂ N	chlornaphazine C142	C ₁₄ H ₂₁ N ₃ O ₄	butralin B232
C ₁₄ H ₁₅ Cl ₂ N ₃ O ₂	etacnazole E55	C ₁₄ H ₂₂ N ₂ O	lignocaine L43
C ₁₄ H ₁₅ N ₃	C.I. Solvent Yellow 3 C424	C ₁₄ H ₂₂ O	<i>tert</i> -octylphenol O23
C ₁₄ H ₁₅ N ₃	<i>N,N</i> -dimethylaminoazobenzene D386	C ₁₄ H ₂₂ O	2,6-di- <i>tert</i> -butylphenol D156
C ₁₄ H ₁₅ N ₃	Methyl Yellow M320	C ₁₄ H ₂₂ O	2,4-di- <i>tert</i> -butylphenol D155
C ₁₄ H ₁₅ N ₅ O ₆ S	metsulfuron-methyl M328	C ₁₄ H ₂₂ O	(2-ethylhexyl)phenol E135
C ₁₄ H ₁₅ O ₂ PS ₂	edifenphos E2	C ₁₄ H ₂₂ O	3,5-di- <i>tert</i> -butylphenol D157
C ₁₄ H ₁₆ ClNO ₃	ofurace O26	C ₁₄ H ₂₃ O ₄ P	dibutyl phenyl phosphate D159
C ₁₄ H ₁₆ ClN ₃ O	metazachlor M98	C ₁₄ H ₂₄ NO ₄ PS ₃	bensulide B36
C ₁₄ H ₁₆ ClO ₅ PS	coumaphos C446	C ₁₄ H ₂₄ N ₂	<i>N,N'</i> -di- <i>sec</i> -butyl- <i>p</i> -phenylenediamine D158
C ₁₄ H ₁₆ F ₃ N ₃ O ₄	profluralin P281		kasugamycin K5
C ₁₄ H ₁₆ N ₂	<i>o</i> -tolidine T172	C ₁₄ H ₂₅ N ₃ O ₉	diisobutyl adipate D351
C ₁₄ H ₁₆ N ₂ O ₂	<i>o</i> -dianisidine D95	C ₁₄ H ₂₆ O ₄	dibutyl adipate D140
C ₁₄ H ₁₆ O	isobutyl 2-naphthyl ether I94	C ₁₄ H ₂₆ O ₄	piperophos P205
C ₁₄ H ₁₇ ClNO ₄ PS ₂	dialifos D68	C ₁₄ H ₂₈ NO ₃ PS ₂	myristyl aldehyde M363
C ₁₄ H ₁₇ Cl ₂ N ₃ O	hexaconazole H43	C ₁₄ H ₂₈ O	myristic acid M362
C ₁₄ H ₁₇ NO ₆	nitrothal-isopropyl N178	C ₁₄ H ₂₈ O ₂	tributyltin acetate T213
C ₁₄ H ₁₇ N ₂ O ₄ PS	pyridaphenthion P355	C ₁₄ H ₃₀ O ₂ Sn	<i>N,N'</i> -dibutylhexamethylenediamine D146
C ₁₄ H ₁₇ O ₅ PS	<i>O,O</i> -diethyl <i>O</i> -(4-methylcoumarin-7-yl) phosphorothioate D309	C ₁₄ H ₃₂ N ₂	fenazaflor F5
C ₁₄ H ₁₈ ClN ₂ O ₃ PS	pyraclofos P347		flucofuron F42
C ₁₄ H ₁₈ ClN ₃ O ₂	triadimenol T197	C ₁₅ H ₇ Cl ₂ F ₃ N ₂ O ₂	anthraflavic acid A219
C ₁₄ H ₁₈ Cl ₂ O ₄	2,4- <i>D</i> , butoxyethanol ester D3	C ₁₅ H ₈ O ₄	coumestrol C449
C ₁₄ H ₁₈ N ₂ O ₄	oxadixyl O45	C ₁₅ H ₈ O ₅	2-methyl-1-nitroanthraquinone M264
C ₁₄ H ₁₈ N ₂ O ₇	dinobuton D504	C ₁₅ H ₉ NO ₄	4 <i>H</i> -cyclopenta[<i>def</i>]phenanthrene C526
C ₁₄ H ₁₈ N ₄ O ₃	benomyl B32		fomesafen F98
C ₁₄ H ₁₈ N ₄ O ₃	trimethoprim T302	C ₁₅ H ₁₀	4,4'-methylenebis(phenyl isocyanate) M214
C ₁₄ H ₁₈ N ₄ O ₄ S ₂	thiophanate T137		isoflavone I104
C ₁₄ H ₁₈ O ₄	dipropyl phthalate D558	C ₁₅ H ₁₀ ClF ₃ N ₂ O ₆ S	flavone F36
C ₁₄ H ₁₈ O ₆	bis(2-methoxyethyl) phthalate B130	C ₁₅ H ₁₀ N ₂ O ₂	daidzein D18
C ₁₄ H ₁₉ Cl ₂ NO ₂	chlorambucil C111		emodin E18
C ₁₄ H ₁₉ NO	ethoxyquin E85	C ₁₅ H ₁₀ O ₂	aloe emodin A95
C ₁₄ H ₁₉ N ₃ S	methapyrilene M117	C ₁₅ H ₁₀ O ₂	genistein G9
C ₁₄ H ₁₉ O ₆ P	α -methylbenzyl 3-hydroxy-crotonate, dimethyl phosphate M167	C ₁₅ H ₁₀ O ₄	quercetin Q2
C ₁₄ H ₂₀ ClNO ₂	acetochlor A14	C ₁₅ H ₁₀ O ₅	oxyfluorfen O59
C ₁₄ H ₂₀ ClNO ₂	alachlor A60	C ₁₅ H ₁₀ O ₅	oxazepam O48
C ₁₄ H ₂₀ ClN ₃ S	methapyrilene hydrochloride M118	C ₁₅ H ₁₀ O ₇	chlorthal-methyl C129
C ₁₄ H ₂₀ N ₂ O	siduron S27	C ₁₅ H ₁₁ ClF ₃ NO ₄	L-thyroxine T156
C ₁₄ H ₂₀ N ₃ O ₅ PS	pyrazophos P350	C ₁₅ H ₁₁ ClO ₃	2,5-diphenyloxazole D548
C ₁₄ H ₂₀ O	lilial L44	C ₁₅ H ₁₁ I ₄ NO ₄	1-amino-2-methylanthraquinone A130
C ₁₄ H ₂₀ O ₂	2,6-di- <i>tert</i> -butyl- <i>p</i> -benzoquinone D144	C ₁₅ H ₁₁ NO	phenytoin sodium P142
		C ₁₅ H ₁₁ NO ₂	nitrazepam N67
		C ₁₅ H ₁₁ N ₂ NaO ₂	
		C ₁₅ H ₁₁ N ₃ O ₃	

C ₁₅ H ₁₂ Br ₄ O ₂	tetrabromobisphenol A T39	C ₁₅ H ₂₃ NO ₄	cycloheximide C513
C ₁₅ H ₁₂ N ₂ O	carbamazepine C61	C ₁₅ H ₂₃ N ₃ O ₄	isopropalin I117
C ₁₅ H ₁₂ N ₂ O ₂	phenytoin P141	C ₁₅ H ₂₄	β-elemene E14
C ₁₅ H ₁₂ O ₅	naringenin N31	C ₁₅ H ₂₄ NO ₄ PS	isofenphos I103
C ₁₅ H ₁₃ NO	2-acetylaminofluorene A23	C ₁₅ H ₂₄ O	nonylphenol (mixed isomers) N198
C ₁₅ H ₁₃ NO ₂	<i>N</i> -hydroxy-2-acetylaminofluorene H109	C ₁₅ H ₂₄ O	4-nonylphenol N197
C ₁₅ H ₁₄ N ₄ O ₂ S	sulfaphenazole S139	C ₁₅ H ₂₄ O	butylated hydroxytoluene B245
C ₁₅ H ₁₄ O ₃	fenoprofen F13	C ₁₅ H ₂₆ N ₂	sparteine S105
C ₁₅ H ₁₄ O ₅	2,2'-dihydroxy-4,4'-dimethoxy-benzophenone D349	C ₁₅ H ₂₆ O ₆	tributyryn T223
C ₁₅ H ₁₅ ClF ₃ N ₃ O	triflumizole T289	C ₁₅ H ₂₇ N ₃ O	2,4,6-tris(dimethylaminomethyl)-phenol T354
C ₁₅ H ₁₅ Cl ₂ N ₃ O ₅	clonitralid C362	C ₁₅ H ₃₃ N	pentadecylamine P33
C ₁₅ H ₁₅ F ₃ N ₂ O ₂	flurprimidol F89	C ₁₅ H ₃₃ N ₃ O ₂	dodine D594
C ₁₅ H ₁₅ NO ₂	mefenamic acid M42	C ₁₅ H ₃₄ BrN	dodecyltrimethylammonium bromide D592
C ₁₅ H ₁₅ N ₃ O ₂	C.I. Disperse Yellow 3 C410	C ₁₆ H ₈ N ₂ Na ₂ O ₈ S ₂	Indigo Carmine I26
C ₁₅ H ₁₅ N ₃ O ₂	Methyl Red M304	C ₁₆ H ₈ N ₂ O ₄	1,6-dinitropyrene D492
C ₁₅ H ₁₆ Cl ₃ N ₃ O ₂	prochloraz P275	C ₁₆ H ₈ N ₂ O ₄	1,8-dinitropyrene D493
C ₁₅ H ₁₆ N ₂ O ₂	ancymidol A207	C ₁₆ H ₉ NO ₂	4-nitropyrene N143
C ₁₅ H ₁₆ N ₄ O ₅ S	sulfometuron-methyl S145	C ₁₆ H ₉ NO ₂	2-nitropyrene N142
C ₁₅ H ₁₆ O ₂	bisphenol A B133	C ₁₆ H ₉ NO ₂	1-nitropyrene N141
C ₁₅ H ₁₇ ClN ₄	myclobutanil M360	C ₁₆ H ₉ NO ₂	3-nitrofluoranthene N113
C ₁₅ H ₁₇ ClN ₄	Neutral Red N42	C ₁₆ H ₁₀	fluoranthene F48
C ₁₅ H ₁₇ Cl ₂ N ₃ O	diniconazole D464	C ₁₆ H ₁₀	pyrene P351
C ₁₅ H ₁₇ Cl ₂ N ₃ O ₂	propiconazole P306	C ₁₆ H ₁₀ N ₂ Na ₂ O ₇ S ₂	C.I. Acid Orange 10 C392
C ₁₅ H ₁₇ N	<i>N</i> -ethyl- <i>N</i> -benzylaniline E100	C ₁₆ H ₁₀ N ₂ Na ₂ O ₇ S ₂	C.I. Food Yellow 3 C415
C ₁₅ H ₁₈ Cl ₂ N ₂ O ₃	oxadiazon O44	C ₁₆ H ₁₀ N ₂ O ₂	Indigo I25
C ₁₅ H ₁₈ Cl ₆ N ₂ O ₅	dichloralphenazone D170	C ₁₆ H ₁₀ S	benzo[<i>b</i>]naphtho[2,3- <i>d</i>]thiophene B67
C ₁₅ H ₁₈ N ₂	4,4'-methylenebis(2-methylaniline) M213	C ₁₆ H ₁₀ S	benzo[<i>b</i>]naphtho[2,1- <i>d</i>]thiophene B66
C ₁₅ H ₁₈ N ₂ O ₆	binapacryl B111	C ₁₆ H ₁₀ S	benzo[<i>b</i>]naphtho[1,2- <i>d</i>]thiophene B65
C ₁₅ H ₁₈ N ₄	ferimzone F31	C ₁₆ H ₁₁ N ₂ NaO ₄ S	C.I. Acid Orange 7 C391
C ₁₅ H ₁₈ N ₄ O ₅	mitomycin M336	C ₁₆ H ₁₂	2-phenylnaphthalene P123
C ₁₅ H ₁₈ N ₆ O ₆ S	ethametsulfuron-methyl E57	C ₁₆ H ₁₂	phenylnaphthalene P122
C ₁₅ H ₁₉ ClN ₄ O ₃	dimefuron D368	C ₁₆ H ₁₂ ClF ₄ N ₃ O ₄	flumetralin F45
C ₁₅ H ₁₉ N ₃ O ₃	imazethapyr I7	C ₁₆ H ₁₂ ClNO ₃	benoxaprofen B34
C ₁₅ H ₂₀ ClN ₃ O	paclobutrazol P1	C ₁₆ H ₁₂ N ₂ O	C.I. Solvent Yellow 14 C426
C ₁₅ H ₂₀ Cl ₂ O ₄	2,4-D, propylene glycol butyl ether ester D15	C ₁₆ H ₁₂ N ₂ O ₄	3,3'-dimethoxybenzidine 4,4'-diisocyanate D379
C ₁₅ H ₂₀ N ₂ O ₄ S	acetohexamide A15	C ₁₆ H ₁₂ O ₂	2-ethylanthraquinone E96
C ₁₅ H ₂₀ O ₆	trimethylolpropane triacrylate T311	C ₁₆ H ₁₃ ClN ₂ O	diazepam D98
C ₁₅ H ₂₁ NO ₄	metalaxyl M93	C ₁₆ H ₁₃ F ₂ N ₃ O	flutriafol F93
C ₁₅ H ₂₁ N ₃ O ₂	physostigmine P178	C ₁₆ H ₁₃ N	<i>N</i> -phenyl-2-naphthylamine P124
C ₁₅ H ₂₂ BrNO	bromobutide B166	C ₁₆ H ₁₄ ClN ₃ O	chlordiazepoxide C120
C ₁₅ H ₂₂ ClNO ₂	metolachlor M323	C ₁₆ H ₁₄ Cl ₂ O ₃	chlorobenzilate C164
C ₁₅ H ₂₂ N ₂ O ₂	4,4'-methylenebis(cyclohexyl isocyanate) M211	C ₁₆ H ₁₄ Cl ₂ O ₄	diclofop-methyl D259
C ₁₅ H ₂₂ O ₃	3,5-di- <i>tert</i> -butyl-4-hydroxybenzoic acid D148	C ₁₆ H ₁₄ N ₂ O	methaqualone M119
C ₁₅ H ₂₃ ClO ₄ S	aramite A232	C ₁₆ H ₁₄ N ₂ O ₂ S	mefenacet M41
C ₁₅ H ₂₃ NO ₃	oxprenolol O52	C ₁₆ H ₁₄ O ₃	ketoprofen K10

C ₁₆ H ₁₄ O ₆	hematoxylin H14	C ₁₆ H ₃₅ N	di- <i>sec</i> -octylamine D515
C ₁₆ H ₁₅ Cl ₃ O ₂	methoxychlor M132	C ₁₆ H ₃₅ O ₄ P	di- <i>sec</i> -octyl phosphate D518
C ₁₆ H ₁₅ FO ₂	fluenetil F44	C ₁₆ H ₃₆ Sn	tetrabutyltin T42
C ₁₆ H ₁₅ F ₂ N ₃ Si	flusilazol F90	C ₁₆ H ₃₇ NO	tetrabutylammonium hydroxide T41
C ₁₆ H ₁₅ NO ₂	cinnamyl anthranilate C347		flubenzimine F40
C ₁₆ H ₁₆ N ₂ O ₂	diacetylbenzidine D67	C ₁₇ H ₁₀ F ₆ N ₄ S	1-methylpyrene M294
C ₁₆ H ₁₆ N ₂ O ₄	desmedipham D59	C ₁₇ H ₁₂	2-methylpyrene M295
C ₁₆ H ₁₆ N ₂ O ₄	phenmedipham P78	C ₁₇ H ₁₂	4-methylpyrene M296
C ₁₆ H ₁₆ O ₂	methoxyphenone M145	C ₁₇ H ₁₂	benzo[<i>a</i>]fluorene B60
C ₁₆ H ₁₇ NO	diphenamid D536	C ₁₇ H ₁₂	nuarimol N209
C ₁₆ H ₁₇ N ₃ O ₄ S	cephalexin C100	C ₁₇ H ₁₂ ClF ₂ N ₂ O	fenarimol F4
C ₁₆ H ₁₈ N ₂ O ₃	difenoxuron D324	C ₁₇ H ₁₂ Cl ₂ N ₂ O	kelevan K6
C ₁₆ H ₁₈ N ₂ O ₄ S	benzylpenicillin B100	C ₁₇ H ₁₂ Cl ₁₀ O ₄	aflatoxin B ₁ A53
C ₁₆ H ₁₈ N ₃ SCl	Methylene Blue M216	C ₁₇ H ₁₂ O ₆	aflatoxin M ₁ A57
C ₁₆ H ₁₈ N ₄ O ₂	nialamide N43	C ₁₇ H ₁₂ O ₇	aflatoxin G ₁ A55
C ₁₆ H ₁₉ N ₃ O ₄ S	ampicillin A194	C ₁₇ H ₁₂ O ₇	Naphthol AS N19
C ₁₆ H ₁₉ N ₃ O ₅ S	amoxycillin A192	C ₁₇ H ₁₃ NO ₂	C.I. Pigment Red 3 C416
C ₁₆ H ₂₀ N ₂	benzathine B45	C ₁₇ H ₁₃ N ₃ O ₃	phthalylsulfathiazole P177
C ₁₆ H ₂₀ N ₂ O ₃	imazamethabenz-methyl I5	C ₁₇ H ₁₃ N ₃ O ₅ S ₂	tefluthrin T15
C ₁₆ H ₂₀ O ₆ P ₂ S ₃	temephos T19	C ₁₇ H ₁₄ ClF ₇ O ₂	ellipticine E15
C ₁₆ H ₂₀ O ₉	gentiopicroin G10	C ₁₇ H ₁₄ N ₂	Oil Orange SS O27
C ₁₆ H ₂₁ HgN ₆ NaO ₇	sodium mercurhydrin S77	C ₁₇ H ₁₄ N ₂ O	benzarone B44
C ₁₆ H ₂₁ NO ₂	propranolol P321	C ₁₇ H ₁₄ O ₃	fumarin F116
C ₁₆ H ₂₂ ClNO ₃	diethatyl-ethyl D282	C ₁₇ H ₁₄ O ₅	aflatoxin B ₂ A54
C ₁₆ H ₂₂ ClN ₃	tripelennamine hydrochloride T334	C ₁₇ H ₁₄ O ₆	aflatoxicol A52
		C ₁₇ H ₁₄ O ₆	aflatoxin G ₂ A56
C ₁₆ H ₂₂ ClN ₃ O	tebuconazole T11	C ₁₇ H ₁₄ O ₇	flamprop-methyl F34
C ₁₆ H ₂₂ Cl ₂ O ₃	2,4-D, octyl ester D14	C ₁₇ H ₁₅ ClFNO ₃	benorylate B33
C ₁₆ H ₂₂ Cl ₂ O ₃	2,4-D, isoctyl ester D10	C ₁₇ H ₁₅ NO ₅	9-hydroxyellipticine H110
C ₁₆ H ₂₂ N ₂ O ₆	aziridyl- <i>p</i> -benzoquinone A267	C ₁₇ H ₁₅ N ₂ O	bromopropylate B187
C ₁₆ H ₂₂ N ₂ O ₇	dinocton D506	C ₁₇ H ₁₆ Br ₂ O ₃	chloropropylate C276
C ₁₆ H ₂₂ O ₄	diisobutyl phthalate D354	C ₁₇ H ₁₆ Cl ₂ O ₃	flutolanil F92
C ₁₆ H ₂₂ O ₄	mono(2-ethylhexyl) phthalate M344	C ₁₇ H ₁₆ F ₃ NO ₂	griseofulvin G46
		C ₁₇ H ₁₇ ClO ₆	benzyl isoeugenol B99
C ₁₆ H ₂₂ O ₄	monoctyl phthalate M346	C ₁₇ H ₁₈ O ₂	fluoxetine hydrochloride F82
C ₁₆ H ₂₂ O ₄	dibutyl phthalate D160	C ₁₇ H ₁₉ ClF ₃ NO	chlorpromazine C310
C ₁₆ H ₂₃ NO ₂	ethoheptazine E73	C ₁₇ H ₁₉ ClN ₂ S	mepronil M58
C ₁₆ H ₂₃ NO ₆	monocrotaline M342	C ₁₇ H ₁₉ NO ₂	morphine M352
C ₁₆ H ₂₃ N ₃ OS	buprofezin B194	C ₁₇ H ₁₉ NO ₃	piperine P203
C ₁₆ H ₂₅ NOS	tiocarbazil T162	C ₁₇ H ₁₉ NO ₃	furalaxyl F119
C ₁₆ H ₂₅ NO ₃	thymoxamine T155	C ₁₇ H ₁₉ NO ₄	fenoxycarb F17
C ₁₆ H ₂₆	decylbenzene D44	C ₁₇ H ₁₉ NO ₄	C.I. Solvent Orange 15 C421
C ₁₆ H ₂₉ N ₃ O ₈	diethylcarbamazine citrate D295	C ₁₇ H ₁₉ N ₃	methyldymron M209
C ₁₆ H ₃₀ O ₄	2,2,4-trimethyl-1,3-pentanediol	C ₁₇ H ₂₀ N ₂ O	dymron D603
	diisobutyrate T316	C ₁₇ H ₂₀ N ₂ O	<i>N,N'</i> -diethylcarbanilide D297
C ₁₆ H ₃₂ O	1,2-epoxyhexadecane E37	C ₁₇ H ₂₀ N ₂ O	4,4'-bis(dimethylamino)-
C ₁₆ H ₃₂ O ₂ Sn	tributyltin methacrylate T218	C ₁₇ H ₂₀ N ₂ O	benzophenone B128
C ₁₆ H ₃₃ NO ₃	lauramide DEA L7		promethazine P287
C ₁₆ H ₃₃ N ₁₁ S ₁₆ Zn ₃	metiram M321	C ₁₇ H ₂₀ N ₂ S	riboflavin R12
C ₁₆ H ₃₄ Cl ₂ Sn	dioctyltin dichloride D523	C ₁₇ H ₂₀ N ₄ O ₆	pentaerythritol tetraacrylate P36
C ₁₆ H ₃₄ O	cetyl alcohol C102	C ₁₇ H ₂₀ O ₈	hexythiazox H80
C ₁₆ H ₃₄ OSn	dioctyltin oxide D526	C ₁₇ H ₂₁ ClN ₂ O ₂ S	

C ₁₇ H ₂₁ ClN ₂ S	promazine hydrochloride P285	C ₁₈ H ₁₅ O ₃ P	triphenyl phosphite T339
C ₁₇ H ₂₁ N	benzphetamine B86	C ₁₈ H ₁₅ O ₄ P	triphenyl phosphate T337
C ₁₇ H ₂₁ NO	diphenhydramine D537	C ₁₈ H ₁₅ P	triphenylphosphine T338
C ₁₇ H ₂₁ NO ₂	napropamide N28	C ₁₈ H ₁₆ ClNO ₅	fenoxaprop-ethyl F16
C ₁₇ H ₂₁ NO ₄	hyoscine H122	C ₁₈ H ₁₆ N ₂ O	C.I. Solvent Orange 7 C420
C ₁₇ H ₂₁ NO ₄ S ₄	bensultap B37	C ₁₈ H ₁₆ N ₂ O ₃	C.I. Solvent Red 80 C423
C ₁₇ H ₂₁ O ₅ PS	coumithoate C450	C ₁₈ H ₁₆ N ₂ O ₆ S	hydroxyquinoline sulfate H120
C ₁₇ H ₂₂ BrNO ₄	hyoscine bromide H123	C ₁₈ H ₁₆ OSn	fentin hydroxide F26
C ₁₇ H ₂₂ ClNO	diphenhydramine hydrochloride D538	C ₁₈ H ₁₇ Cl ₂ NO ₃	benzoylprop-ethyl B84
C ₁₇ H ₂₂ ClN ₃	auramine A254	C ₁₈ H ₁₈ ClNO ₅	benzoximate B81
C ₁₇ H ₂₂ N ₂	4,4'-methylenebis(<i>N,N</i> -dimethylaniline) M212	C ₁₈ H ₁₈ N ₆	Bandrowski's base B2
C ₁₇ H ₂₂ N ₂ O	doxylamine D598	C ₁₈ H ₁₈ O ₃	flurenol-butyl F85
C ₁₇ H ₂₃ NO ₃	hyoscyamine H124	C ₁₈ H ₂₀ Cl ₂	1,1-dichloro-2,2-bis(4-ethylphenyl)ethane D199
C ₁₇ H ₂₃ NO ₃	atropine A253	C ₁₈ H ₂₀ N ₂ O ₄ S	difenzoquat metilsulfate D325
C ₁₇ H ₂₄ NNaO ₅	alloxym-dim-sodium A71	C ₁₈ H ₂₀ O ₂	stilbestrol S116
C ₁₇ H ₂₄ O ₃	cyclandelate C496	C ₁₈ H ₂₀ O ₂	equilin E41
C ₁₇ H ₂₅ N ₃ O ₄ S ₂	alanycarb A61	C ₁₈ H ₂₂ Cl ₂ N ₂	chlorocyclizine hydrochloride C188
C ₁₇ H ₂₆ ClNO ₂	butachlor B196	C ₁₈ H ₂₂ N ₂	cyclizine C497
C ₁₇ H ₂₆ N ₈ O ₅	blasticidin-S B139	C ₁₈ H ₂₂ N ₂ O ₁₂	nicotine tartrate N56
C ₁₇ H ₂₉ NO ₃ S	sethoxym S25	C ₁₈ H ₂₂ O ₂	estrone E53
C ₁₇ H ₃₀ ClN	laurylpyridinium chloride L10	C ₁₈ H ₂₂ O ₂	dicumyl peroxide D264
C ₁₇ H ₃₀ O ₂	hydroprene H106	C ₁₈ H ₂₂ O ₅	zearalenone Z1
C ₁₇ H ₃₄ O ₄	1,1-bis(<i>tert</i> -butylperoxy)-3,3,5-trimethylcyclohexane B117	C ₁₈ H ₂₃ Cl ₂ NO	phenoxybenzamine hydrochloride P85
C ₁₇ H ₃₈ NBr	myristyltrimethylammonium bromide M364	C ₁₈ H ₂₃ NO	orphenadrine O35
C ₁₈ H ₁₀	benzo[ghi]fluoranthene B57	C ₁₈ H ₂₃ NO ₃	dihydrocodeine D344
C ₁₈ H ₁₁ NO ₂	6-nitrochrysene N102	C ₁₈ H ₂₃ NO ₆	ridelline R14
C ₁₈ H ₁₂	benz[a]anthracene B43	C ₁₈ H ₂₄ NO ₇ P	codeine phosphate C383
C ₁₈ H ₁₂	chrysene C340	C ₁₈ H ₂₄ N ₂ O ₆	dinocap D505
C ₁₈ H ₁₂	naphthacene N6	C ₁₈ H ₂₄ O ₂	α-estradiol E51
C ₁₈ H ₁₂	triphenylene T336	C ₁₈ H ₂₄ O ₂	estradiol E50
C ₁₈ H ₁₂ CaClN ₂ O ₆ S	C.I. Pigment Red 48:2 C418	C ₁₈ H ₂₄ O ₃	oestriol O25
C ₁₈ H ₁₂ CuN ₂ O ₂	oxine-copper O50	C ₁₈ H ₂₅ NO	dextromethorphan D63
C ₁₈ H ₁₂ O ₆	sterigmatocystin S114	C ₁₈ H ₂₆ ClN ₃	chloroquine C281
C ₁₈ H ₁₃ ClF ₃ NO ₇	fluoroglycofen-ethyl F66	C ₁₈ H ₂₆ NOBr	dextromethorphan hydrobromide D64
C ₁₈ H ₁₃ NO ₃	naptalam N30	C ₁₈ H ₂₆ N ₂ O ₅ S	furathiocarb F125
C ₁₈ H ₁₃ N ₄ NaO ₇ S	C.I. Acid Orange 3 C390	C ₁₈ H ₂₆ O	galaxolide G2
C ₁₈ H ₁₄	<i>m</i> -terphenyl T29	C ₁₈ H ₂₆ O ₄	dipentyl phthalate D534
C ₁₈ H ₁₄	<i>p</i> -terphenyl T31	C ₁₈ H ₂₆ O ₆	trimethylolpropane trimethacrylate T312
C ₁₈ H ₁₄	<i>o</i> -terphenyl T30	C ₁₈ H ₂₈ O ₃ S	sulfoxide S148
C ₁₈ H ₁₄	terphenyl T28	C ₁₈ H ₂₉ NaO ₃ S	sodium dodecylbenzenesulfonate S65
C ₁₈ H ₁₄ Cl ₄ N ₂ O	miconazole M332	C ₁₈ H ₃₀	1-phenyldodecane P100
C ₁₈ H ₁₄ N ₂ Na ₂ O ₇ S ₂	C.I. Acid Red 26 C395	C ₁₈ H ₃₀ O	dodecylphenol D591
C ₁₈ H ₁₄ N ₄ O ₅ S	sulfasalazine S140	C ₁₈ H ₃₀ O	2,4,6- <i>tert</i> -butylphenol T211
C ₁₈ H ₁₅ ClN ₄	phenosafranin P82	C ₁₈ H ₃₀ O ₃ S	dodecylbenzenesulfonic acid D589
C ₁₈ H ₁₅ ClSn	triphenyltin chloride T340	C ₁₈ H ₃₂ O ₂	linoleic acid L49
C ₁₈ H ₁₅ ClSi	chlorotriphenylsilane C305		
C ₁₈ H ₁₅ FSn	triphenyltin fluoride T341		
C ₁₈ H ₁₅ N	triphenylamine T335		

C ₁₈ H ₃₃ ClN ₂ O ₅ S	clindamycin C354	C ₁₉ H ₂₁ ClN ₂ O	pencycuron P19
C ₁₈ H ₃₄ OSn	cyhexatin C535	C ₁₉ H ₂₂ N ₂ O	vinburnine V22
C ₁₈ H ₃₄ O ₂	(Z)-oleic acid O31	C ₁₉ H ₂₂ O ₆	gibberellic acid G14
C ₁₈ H ₃₄ O ₂	(E)-oleic acid O30	C ₁₉ H ₂₃ ClN ₂ O ₂ S	pyridate P356
C ₁₈ H ₃₄ O ₆	di-sec-octyl peroxydicarbonate D517	C ₁₉ H ₂₃ NO ₃	ethylmorphine E151
		C ₁₉ H ₂₃ N ₃	amitraz A158
C ₁₈ H ₃₆	dodecylcyclohexane D590	C ₁₉ H ₂₄ N ₂	imipramine I14
C ₁₈ H ₃₆ BrN	piroctanyl bromide P206	C ₁₉ H ₂₄ O ₃	prallethrin P267
C ₁₈ H ₃₆ O ₂	stearic acid S112	C ₁₉ H ₂₅ ClN ₂	imipramine hydrochloride I15
C ₁₈ H ₃₆ O ₇	sorbitan monolaurate S103	C ₁₉ H ₂₅ NO ₄	tetramethrin T85
C ₁₈ H ₃₇ Cl ₃ Si	octadecyltrichlorosilane O4	C ₁₉ H ₂₆ O ₃	allethrin A68
C ₁₈ H ₃₇ N	oleamine O28	C ₁₉ H ₂₆ O ₄ S	propargite P300
C ₁₈ H ₃₈ NO ₃ P	buminafos B192	C ₁₉ H ₂₇ NO	pentazocine P42
C ₁₈ H ₃₈ O	stearyl alcohol S113	C ₁₉ H ₂₇ NO ₆	senkirkine S23
C ₁₈ H ₃₈ S	1-octadecanethiol O3	C ₁₉ H ₂₈ O ₂	testosterone T38
C ₁₈ H ₃₉ N	stearamine S111	C ₁₉ H ₃₀ O ₅	piperonyl butoxide P204
C ₁₈ H ₃₉ O ₇ P	tris(2-butoxyethanol) phosphate T348	C ₁₉ H ₃₁ N	fenpropidin F19
		C ₁₉ H ₃₂ Cl ₃ P	chlorphonium chloride C309
C ₁₈ H ₃₉ SiCl	chlorotrihexylsilane C303	C ₁₉ H ₃₂ O ₂ Sn	tributyltin benzoate T214
C ₁₈ H ₄₁ N ₇	iminotadine I10	C ₁₉ H ₃₄ O ₃	methoprene M127
C ₁₈ H ₄₂ OSn ₂	tripropyltin oxide T344	C ₁₉ H ₃₆ O ₂	Z-methyl oleate M270
C ₁₉ H ₁₁ F ₅ N ₂ O ₂	diflufenican D327	C ₁₉ H ₃₇ N	nonadecanenitrile N191
C ₁₉ H ₁₂ O ₂	β-naphthoflavone N14	C ₁₉ H ₃₉ NO(appr	tridemorph T273
C ₁₉ H ₁₂ O ₂	α-naphthoflavone N13	C ₁₉ H ₄₂ BrN	cetyltrimethylammonium bromide C105
C ₁₉ H ₁₂ O ₆	dicoumarin D262		Rose Bengal sodium R16
C ₁₉ H ₁₄	3-methylchrysene M193	C ₂₀ H ₄ Cl ₄ I ₄ Na ₂ O ₅	eosin E29
C ₁₉ H ₁₄	2-methylchrysene M192	C ₂₀ H ₆ Br ₄ Na ₂ O ₅	C.I. Acid Yellow 73 C399
C ₁₉ H ₁₄	5-methylchrysene M194	C ₂₀ H ₁₀ Na ₂ O ₅	Amaranth A108
C ₁₉ H ₁₄	1-methylchrysene M191	C ₂₀ H ₁₁ N ₂ Na ₃ O ₁₀ S ₃	benzo[a]pyrene B71
C ₁₉ H ₁₄	6-methylchrysene M195	C ₂₀ H ₁₂	benzo[b]fluoranthene B56
C ₁₉ H ₁₄ F ₃ NO	fluridone F86	C ₂₀ H ₁₂	benzo[k]fluoranthene B59
C ₁₉ H ₁₅ Cl	trityl chloride T363	C ₂₀ H ₁₂	benzo[j]fluoranthene B58
C ₁₉ H ₁₅ ClO ₄	coumachlor C445	C ₂₀ H ₁₂	perylene P57
C ₁₉ H ₁₅ NaO ₄	warfarin sodium W3	C ₂₀ H ₁₂	benzo[e]pyrene B72
C ₁₉ H ₁₆ ClNO ₄	indomethacin I35	C ₂₀ H ₁₂	C.I. Acid Red 14 C393
C ₁₉ H ₁₆ N ₂ Na ₂ O ₇ S ₂	C.I. Food Red 6 C414	C ₂₀ H ₁₂ N ₂ Na ₂ O ₇ S ₂	fluorescein F51
C ₁₉ H ₁₆ O ₃	coumatetralyl C448	C ₂₀ H ₁₂ O ₅	7H-dibenzo[c,g]carbazole D104
C ₁₉ H ₁₆ O ₄	(+)-warfarin W2	C ₂₀ H ₁₃ N	C.I. Acid Red 88 C397
C ₁₉ H ₁₆ O ₄	warfarin W1	C ₂₀ H ₁₃ N ₂ NaO ₄ S	C.I. Acid Red 18 C394
C ₁₉ H ₁₇ ClFN ₃ O ₅ S	flucloxacillin F41	C ₂₀ H ₁₄ N ₂ Na ₃ O ₁₀ S ₃	diphenyl phthalate D549
C ₁₉ H ₁₇ ClN ₂ O ₄	quizalofop-ethyl Q13	C ₂₀ H ₁₄ O ₄	phenolphthalein P81
C ₁₉ H ₁₈ ClN ₃	C.I. Basic Red 9 C402	C ₂₀ H ₁₄ O ₄	5,6-dimethylchrysene D408
C ₁₉ H ₁₉ ClFN ₃ O ₃	flamprop-M-isopropyl F35	C ₂₀ H ₁₆	7,12-dimethylbenz[a]anthracene D401
C ₁₉ H ₁₉ ClF ₃ NO ₅	haloxyfop-ethoxyethyl H5	C ₂₀ H ₁₆	ochratoxin A O1
C ₁₉ H ₁₉ N ₇ O ₆	folic acid F96		fentin acetate F25
C ₁₉ H ₂₀ F ₃ NO ₄	fluzafop-P-butyl F39	C ₂₀ H ₁₈ ClNO ₆	acronycine A40
C ₁₉ H ₂₀ F ₃ NO ₄	fluzafop-butyl F38	C ₂₀ H ₁₈ O ₂ Sn	dichloromethotrexate D223
C ₁₉ H ₂₀ N ₂	mebhydrolin M36	C ₂₀ H ₁₉ NO ₃	feprazone F29
C ₁₉ H ₂₀ N ₂ O ₂	phenylbutazone P96	C ₂₀ H ₂₀ Cl ₂ N ₈ O ₅	Magenta I M1
C ₁₉ H ₂₀ N ₂ O ₃	oxyphenbutazone O63	C ₂₀ H ₂₀ N ₂ O ₂	papaverine P4
C ₁₉ H ₂₀ N ₈ O ₅	aminopterin A150	C ₂₀ H ₂₀ N ₃ Cl	
C ₁₉ H ₂₀ O ₄	benzyl butyl phthalate B94	C ₂₀ H ₂₁ NO ₄	

$C_{20}H_{22}ClNO_4$	papaverine hydrochloride P5	$C_{21}H_{22}Cl_2N_2O_8$	demeclocycline hydrochloride D48
$C_{20}H_{22}N_2O$	fenazaquin F6		strychnine S125
$C_{20}H_{22}N_8O_5$	methotrexate M128	$C_{21}H_{22}N_2O_2$	barbaloin B3
$C_{20}H_{22}O_3$	nafenopin N2	$C_{21}H_{22}O_9$	flurazepam F84
$C_{20}H_{23}ClN_2O_4$	chlorpheniramine maleate C308	$C_{21}H_{23}ClFN_3O$	bisphenyl A diglycidyl ether B134
$C_{20}H_{23}N$	amitriptyline A159	$C_{21}H_{24}O_4$	D-glucine G15
$C_{20}H_{23}NO_3$	benalaxyl B26	$C_{21}H_{25}NO_4$	(+)-yohimbine Y1
$C_{20}H_{23}N_3O_2$	bitertanol B137	$C_{21}H_{26}N_2O_3$	thioridazine T143
$C_{20}H_{24}ClN_3S$	prochlorperazine P276	$C_{21}H_{26}N_2S_2$	mestranol M92
$C_{20}H_{24}N_2O_2$	quinine Q6	$C_{21}H_{26}O_2$	clivorine C355
$C_{20}H_{24}N_2O_2S$	hycanthone H84	$C_{21}H_{28}NO_7$	doxylamine succinate D599
$C_{20}H_{24}O_2$	ethinyloestradiol E66	$C_{21}H_{28}N_2O_5$	buthiobate B221
$C_{20}H_{26}N_2$	trimipramine T328	$C_{21}H_{28}N_2S_2$	levonorgestrel L38
$C_{20}H_{26}O_2$	norethisterone N204	$C_{21}H_{28}O_2$	pyrethrin I P352
$C_{20}H_{26}O_2$	norethynodrel N205	$C_{21}H_{28}O_3$	cinerin II C345
$C_{20}H_{26}O_4$	dicyclohexyl phthalate D268	$C_{21}H_{28}O_5$	prednisolone P269
$C_{20}H_{28}NBr$	emepromium bromide E16	$C_{21}H_{28}O_5$	fluorocortisone F63
$C_{20}H_{28}O$	lynestrenol L67	$C_{21}H_{29}FO_5$	progesterone P282
$C_{20}H_{28}O_2$	isotretinoin I138	$C_{21}H_{30}O_2$	hydroxyprogesterone H115
$C_{20}H_{28}O_3$	cinerin I C344	$C_{21}H_{30}O_3$	jasmolin I J1
$C_{20}H_{28}O_6$	phorbol P146	$C_{21}H_{30}O_3$	hydrocortisone H95
$C_{20}H_{30}N_2O_5S$	benfuracarb B30	$C_{21}H_{30}O_5$	pregnenolone P270
$C_{20}H_{30}O$	retinol R7	$C_{21}H_{32}O_2$	oxymetholone O62
$C_{20}H_{30}O$	vitamin A V40	$C_{21}H_{32}O_3$	lasiocarpine L6
$C_{20}H_{30}O_2$	abietic acid A2	$C_{21}H_{33}NO_7$	cetylpyridinium chloride C104
$C_{20}H_{30}O_4$	dihexyl phthalate D341	$C_{21}H_{38}NCl$	glycidyl oleate G34
$C_{20}H_{30}O_6$	bis(2-butoxyethyl) phthalate B116	$C_{21}H_{38}O_3$	hexetidine H75
	carbosulfan C83	$C_{21}H_{45}N_3$	indeno[1,2,3- <i>cd</i>]pyrene I24
$C_{20}H_{32}N_2O_3S$	ephedrine sulfate E31	$C_{22}H_{12}$	dibenzo[<i>cd,jk</i>]pyrene D119
$C_{20}H_{32}N_2O_6S$	nicotine sulfate N55	$C_{22}H_{12}$	benzo[<i>ghi</i>]perylene B69
$C_{20}H_{32}N_4O_4S$	arachidonic acid A231	$C_{22}H_{12}$	dibenz[<i>a,h</i>]anthracene D103
$C_{20}H_{32}O_2$	fenpropimorph F20	$C_{22}H_{14}$	fluotrimazole F81
$C_{20}H_{33}NO$	1,4-di(<i>tert</i> -butylperoxyisopropyl)-benzene D154	$C_{22}H_{16}F_3N_3$	C.I. Solvent Red 23 C422
$C_{20}H_{34}O_4$	azocyclotin A270	$C_{22}H_{16}N_4O$	clotrimazole C365
	diocetyltn maleate D525	$C_{22}H_{17}ClN_2$	cyfluthrin C533
$C_{20}H_{35}N_3Sn$	docusate sodium D583	$C_{22}H_{18}Cl_2FNO_3$	deltamethrin D46
$C_{20}H_{36}O_4Sn$	dodemorph acetate D593	$C_{22}H_{19}Br_2NO_3$	tralomethrin T194
$C_{20}H_{38}O_7SNa$	selenium diethylidithiocarbamate S15	$C_{22}H_{19}Br_4NO_3$	α -cypermethrin C543
$C_{20}H_{39}NO_3$	ethyl tellurac E174	$C_{22}H_{19}Cl_2NO_3$	cypermethrin C542
$C_{20}H_{40}N_4S_8Se$	eicosanoic acid E13	$C_{22}H_{19}Cl_2NO_3$	carminic acid C86
	dibenz[<i>a,j</i>]acridine D102	$C_{22}H_{20}O_{13}$	propaquizafop P299
$C_{20}H_{40}O_2$	dibenz[<i>a,h</i>]acridine D101	$C_{22}H_{22}ClN_3O_5$	7-chlortetracycline C316
$C_{21}H_{13}N$	3-methylcholanthrene M190	$C_{22}H_{23}ClN_2O_8$	fenpropathrin F18
$C_{21}H_{13}N$	ethidium bromide E65	$C_{22}H_{23}NO_3$	tetracycline T62
$C_{21}H_{16}$	permethrin P56	$C_{22}H_{24}N_2O_8$	oxytetracycline O64
$C_{21}H_{20}BrN_3$	curcumin C478	$C_{22}H_{24}N_2O_9$	colchicine C384
$C_{21}H_{20}Cl_2O_3$	demeclocycline D47	$C_{22}H_{25}NO_6$	resmethrin R4
$C_{21}H_{20}O_6$	tri- <i>o</i> -tolyl phosphate T362	$C_{22}H_{26}O_3$	physostigmine salicylate P179
$C_{21}H_{21}ClN_2O_8$	tritoyl phosphate T361	$C_{22}H_{27}N_3O_5$	tebufenozide T12
$C_{21}H_{21}O_4P$		$C_{22}H_{28}N_2O_2$	pyrethrin II P353
$C_{21}H_{21}O_4P$		$C_{22}H_{28}O_5$	dexamethasone D62
		$C_{22}H_{29}FO_5$	

$C_{22}H_{29}NO_2$	levopropoxyphene L39	$C_{24}H_{32}O_4$	ethynodiol diacetate E182
$C_{22}H_{29}NO_2$	propoxyphene P318	$C_{24}H_{32}O_4$	megestrol acetate M44
$C_{22}H_{30}Cl_2N_{10}$	chlorhexidine C130	$C_{24}H_{32}O_4S$	spironolactone S108
$C_{22}H_{30}NO_2Cl$	propoxyphene hydrochloride P319	$C_{24}H_{38}O_4$	di- <i>n</i> -octyl phthalate D520
$C_{22}H_{30}O_2S$	4,4'-thiobis(5- <i>tert</i> -butyl- <i>m</i> -cresol) T118	$C_{24}H_{38}O_4$	dioctyl phthalate D519
$C_{22}H_{30}O_2S$	4,4'-thiobis(5- <i>tert</i> -butyl- <i>o</i> -cresol) T119	$C_{24}H_{40}O_3$	lithocholic acid L56
$C_{22}H_{30}O_5$	jasmolin II J2	$C_{24}H_{40}O_8$	pirotal P207
$C_{22}H_{34}O_4$	diheptyl phthalate D340	$C_{24}H_{42}O$	2,4-dinonylphenol D507
$C_{22}H_{42}O_4$	di- <i>n</i> -octyl adipate D513	$C_{24}H_{46}O_4$	lauroyl peroxide L9
$C_{22}H_{42}O_4$	di- <i>sec</i> -octyl adipate D514	$C_{24}H_{50}O_2Sn$	tributyltin laurate T217
$C_{22}H_{42}O_6$	bis(2-hexyloxyethyl) adipate B129	$C_{24}H_{51}O_4P$	tris(2-ethylhexyl) phosphate T355
$C_{22}H_{42}O_8$	dibutoxyethoxyethyl adipate D139	$C_{24}H_{51}O_4P$	trioctyl phosphate T332
$C_{22}H_{43}NO$	erucamide E46	$C_{24}H_{54}OSn_2$	tributyltin oxide T219
$C_{22}H_{46}N_2O$	2-heptadecyl-2-imidazoline-1-ethanol H17	$C_{24}H_{54}SSn_2$	tributyltin sulfide T222
$C_{22}H_{48}NCl$	didecyl dimethylammonium chloride D274	$C_{25}H_{22}ClNO_3$	fenvalerate F28
$C_{23}H_{14}Na_2O_{11}$	sodium chromoglycate S57	$C_{25}H_{22}ClNO_3$	esfenvalerate E49
$C_{23}H_{15}ClO_3$	chlorophacinone C238	$C_{25}H_{24}F_6N_4$	hydramethylnon H86
$C_{23}H_{16}O_3$	diphacinone D535	$C_{25}H_{35}NO_5$	mebeverine M35
$C_{23}H_{19}ClF_3NO_3$	cyhalothrin C534	$C_{25}H_{46}ClN$	cetyldimethylbenzylammonium chloride C103
$C_{23}H_{21}ClO_3$	chlorotrianisene C299	$C_{26}H_{22}ClF_3N_2O_3$	τ -fluvalinate F94
$C_{23}H_{22}ClF_3O_2$	bifenthrin B109	$C_{26}H_{23}F_2NO_4$	flucythrinate F43
$C_{23}H_{22}O_6$	rotenone R18	$C_{26}H_{28}Cl_2N_4O_4$	ketoconazole K9
$C_{23}H_{23}IN_2S_2$	dithiazanine iodide D571	$C_{26}H_{29}NO$	tamoxifen T5
$C_{23}H_{24}O_4S$	kadethrin K1	$C_{26}H_{42}O_4$	octyl decyl phthalate O22
$C_{23}H_{25}ClN_2$	Malachite Green M9	$C_{26}H_{42}O_4$	dinonyl phthalate D508
$C_{23}H_{26}N_2O_4$	brucine B191	$C_{27}H_{26}N_2O_7S_2Na$	C.I. Acid Green 50 C389
$C_{23}H_{26}O_3$	phenothrin P84	$C_{27}H_{29}NO_{10}$	daunomycin D23
$C_{23}H_{29}ClO_4$	chlormadinone acetate C139	$C_{27}H_{29}NO_{11}$	doxorubicin D596
$C_{23}H_{30}ClN_3O$	mepacrine M55	$C_{27}H_{29}N_2NaO_7S_2$	C.I. Acid Red 52 C396
$C_{23}H_{30}O_3$	etretinate E184	$C_{27}H_{30}ClNO_{11}$	doxorubicin hydrochloride D597
$C_{23}H_{45}N_5O_{14}$	neomycin E N38	$C_{27}H_{30}O_{16}$	rutin R22
$C_{23}H_{46}N_6O_{13}$	neomycin C N37	$C_{27}H_{31}N_2NaO_6S_2$	C.I. Acid Blue 1 C386
$C_{23}H_{46}N_6O_{13}$	neomycin B N36	$C_{27}H_{34}N_2O_4S$	C.I. Basic Green 1 C400
$C_{24}H_{12}O_2$	C.I. Vat Yellow 4 C428	$C_{27}H_{42}NO_2Cl$	benzethonium chloride B51
$C_{24}H_{14}$	dibenzo[<i>a,e</i>]pyrene D115	$C_{27}H_{44}O$	cholecalciferol C323
$C_{24}H_{14}$	dibenzo[<i>a,h</i>]pyrene D116	$C_{27}H_{44}O_7$	β -ecdysterone E1
$C_{24}H_{14}$	dibenzo[<i>a,i</i>]pyrene D117	$C_{27}H_{46}O$	cholesterol C324
$C_{24}H_{14}$	dibenzo[<i>a,l</i>]pyrene D118	$C_{27}H_{50}O_6$	tricaprylin T224
$C_{24}H_{16}As_2O_3$	10,10'-oxybisphenoxarsine O55	$C_{28}H_{31}ClN_2O_3$	C.I. Basic Red 1 C401
$C_{24}H_{17}N_5O_7$	C.I. Pigment Red 23 C417	$C_{28}H_{31}ClN_2O_3$	rhodamine B R9
$C_{24}H_{26}N_2O_{13}$	Beetroot Red B25	$C_{28}H_{34}O_{15}$	hesperidine H30
$C_{24}H_{26}N_2O_{13}$	betanin B107	$C_{28}H_{40}N_2O_9$	antimycin A A228
$C_{24}H_{27}N$	prenylamine P271	$C_{28}H_{43}N$	4,4'-dioctyldiphenylamine D516
$C_{24}H_{27}N_3O_4$	fenpyroximate F21	$C_{28}H_{44}O$	ergocalciferol E42
$C_{24}H_{28}O_4$	stilbestrol dipropionate S117	$C_{28}H_{44}O$	ergosterol E43
$C_{24}H_{28}O_8$	stilbestrol monoglucuronide S118	$C_{28}H_{46}O_4$	didecyl phthalate D275
		$C_{28}H_{46}O_4$	diisodecyl phthalate D355
		$C_{28}H_{56}O_4Sn_2$	tributyltin fumarate T216
		$C_{28}H_{58}O_4Sn_2$	tributyltin succinate T221
		$C_{29}H_{38}N_4O_{10}$	lymecycline L66
		$C_{29}H_{42}Cl_2N_2O_4$	emetine hydrochloride E17

$C_{29}H_{44}O_{12}$	ouabain O40	$C_{36}H_{70}O_4Zn$	zinc stearate Z16
$C_{29}H_{50}O_2$	α -tocopherol T169	$C_{36}H_{72}O_4S_2Sn$	dioctyltin bis(2-ethylhexyl thioglycolate) D521
$C_{30}H_{23}BrO_4$	bromadiolone B152		dioctyltin bis(isooctyl thioglycolate) D522
$C_{30}H_{34}O_{13}$	picrotoxin P188	$C_{36}H_{72}O_4S_2Sn$	C.I. Acid Red 114 C398
$C_{30}H_{44}O_9$	cymarin C536		C.I. Food Blue 2 C411
$C_{30}H_{50}$	squalene S109	$C_{37}H_{28}N_4Na_2O_{10}S_3$	C.I. Food Green 3 C412
$C_{30}H_{50}O_2$	diundecyl phthalate D578	$C_{37}H_{34}N_2Na_2O_9S_3$	C.I. Acid Green 3 C388
$C_{30}H_{58}O_4S$	dilauryl 3,3'-thiodipropionate D365	$C_{37}H_{36}N_2NaO_6S_2$	C.I. Acid Blue 9 C387
$C_{31}H_{18}CuN_6Na_2O_9S$	C.I. Direct Brown 95 C407	$C_{37}H_{36}N_2O_9S_3Na_2$	erythromycin E47
$C_{31}H_{23}BrO_3$	brodifacoum B150	$C_{37}H_{67}NO_{13}$	Benzyl Violet 4B B101
$C_{31}H_{24}O_3$	difenacoum D323	$C_{39}H_{40}N_3O_6S_2Na$	phenesterine P65
$C_{31}H_{46}O_2$	phytomenadione P181	$C_{39}H_{59}Cl_2NO_2$	C.I. Food Orange 8 C413
$C_{32}H_{16}CuN_8$	phthalocyanine blue P176	$C_{40}H_{52}O_2$	α -carotene C88
$C_{32}H_{16}Cu_2N_6Na_4O_{16}S_4$	C.I. Direct Blue 218 C406	$C_{40}H_{56}$	γ -carotene C90
$C_{32}H_{20}N_6Na_4O_{14}S_4$	C.I. Direct Blue 6 C404	$C_{40}H_{56}$	β -carotene C89
$C_{32}H_{26}Cl_2NO_4$	Diarylanilide Yellow D96	$C_{40}H_{56}$	lycopene L65
$C_{32}H_{26}N_4Na_2O_8S_2$	C.I. Direct Red 39 C408	$C_{40}H_{56}O_3$	capsanthin C56
$C_{32}H_{36}ClNO_8$	clomiphene citrate C361	$C_{40}H_{56}O_4$	capsorubin C57
$C_{32}H_{37}NO_5S$	propoxyphene napsylate P320	$C_{40}H_{80}O_4Sn$	dioctyltin dilaurate D524
$C_{32}H_{38}N_2O_8$	deserpidine D58	$C_{41}H_{64}O_{13}$	digitoxin D335
$C_{32}H_{44}O_{12}$	scilliroside S10	$C_{41}H_{64}O_{14}$	digoxin D339
$C_{32}H_{54}O_4$	dilauryl phthalate D364	$C_{42}H_{30}N_6O_{12}$	inositol niacinate I38
$C_{32}H_{58}O_4Sn_2$	tributyltin phthalate T220	$C_{42}H_{50}Cl_4N_2O_4$	estradiol mustard E52
$C_{32}H_{64}O_4Sn$	dibutyltin dilaurate D163	$C_{42}H_{70}O_{35}$	β -cyclodextrin C501
$C_{33}H_{25}F_3O_4$	flocoumafen F37	$C_{43}H_{47}N_2NaO_6S_2$	Indocyanine Green I30
$C_{33}H_{25}N_3O_3$	norbormide N201	$C_{43}H_{58}N_4O_{12}$	rifampicin R15
$C_{33}H_{40}N_2O_9$	reserpine R3	$C_{45}H_{58}O_6C_{21}$	ovulen O41
$C_{33}H_{47}NO_{13}$	pimaricin P191	$C_{46}H_{56}N_4O_{10}$	vincristine V24
$C_{34}H_{24}N_6Na_4O_{14}S_4$	Evans Blue E190	$C_{46}H_{58}N_4O_9$	vinblastine V20
$C_{34}H_{24}N_6Na_4O_{14}S_4$	Trypan Blue T366	$C_{46}H_{58}N_4O_{14}S$	vincristine sulfate V25
$C_{34}H_{26}BaCl_2N_4O_8S_2$	D & C Red 9 D27	$C_{46}H_{60}N_4O_{13}S$	vinblastine sulfate V21
$C_{34}H_{27}N_9Na_2O_7S_2$	C.I. Direct Black 38 C403	$C_{47}H_{75}NO_{17}$	nystatin N210
$C_{34}H_{28}N_6Na_4O_{16}S_4$	C.I. Direct Blue 15 C405	$C_{48}H_{56}N_6O_8S_2$	benzathine penicillin B46
$C_{34}H_{32}MgN_4O_7$	chlorophyllin b C258	$C_{48}H_{80}O_{40}$	γ -cyclodextrin C502
$C_{34}H_{33}FeN_4O_5$	hematin H12	$C_{54}H_{70}MgN_4O_6$	chlorophyll d C256
$C_{34}H_{34}MgN_4O_6$	chlorophyllin a C257	$C_{54}H_{90}N_6O_{18}$	valinomycin V7
$C_{34}H_{38}N_4O_6$	hematoporphyrin H13	$C_{55}H_{70}MgN_4O_6$	chlorophyll b C254
$C_{34}H_{38}O_4$	ditridecyl phthalate D577	$C_{55}H_{72}MgN_4O_5$	chlorophyll a C253
$C_{34}H_{47}NO_{11}$	aconitine A33	$C_{60}H_{78}OSn_2$	fenbutatin oxide F7
$C_{34}H_{58}O_4$	diisotridecyl phthalate D361	$C_{61}H_{122}O_{24}$	polysorbate 80 P230
$C_{34}H_{63}N_5O_9$	pepstatin A P50	$C_{62}H_{86}N_{12}O_{16}$	actinomycin D A46
$C_{35}H_{30}MgN_4O_5$	chlorophyll c C255	$C_{62}H_{86}N_{12}O_{16}$	actinomycin C A45
$C_{35}H_{44}O_{16}$	azadirachtin A258	$C_{62}H_{111}N_{11}O_{12}$	cyclosporin A C531
$C_{35}H_{61}NO_{12}$	oleandomycin O29	$C_{62}H_{122}O_{26}$	polysorbate 40 P228
$C_{36}H_{34}Cl_2N_6O_4$	C.I. Pigment Yellow 13 C419	$C_{63}H_{88}CoN_{14}O_{14}P$	cobalamin C368
$C_{36}H_{58}CaO_6S_2$	calcium dodecylbenzenesulfonate C32	$C_{66}H_{103}N_{17}O_{16}S$	bacitracin B1
$C_{36}H_{60}O_{30}$	α -cyclodextrin C500	$C_{70}H_{76}N_{10}O_{16}$	ergotamine tartrate E44
$C_{36}H_{66}O_4Hg$	mercury oleate M80	$C_{76}H_{52}O_{46}$	tannic acid T6
$C_{36}H_{70}O_4Cd$	cadmium stearate C12	$C_{88}H_{124}CoO_8$	cobalt resinate C377
$C_{36}H_{70}O_4Pb$	lead distearate L20	$C_{132}H_{189}AlO_{15}$	aluminium resinate A106

Ca	calcium C21	Cl ₂	chlorine C135
CaC ₂	calcium carbide C24	Cl ₂ Cr	chromium(II) chloride C333
CaCl ₂ O ₂	calcium hypochlorite C34	Cl ₂ CrO ₂	chromyl chloride C339
CaCl ₂ O ₄	calcium chlorite C27	Cl ₂ Cu	copper(II) chloride C434
CaCl ₂ O ₆	calcium chlorate C26	Cl ₂ CuO ₆	copper chlorate C432
CaCrO ₄	calcium chromate C28	Cl ₂ Fe	iron(II) chloride I68
CaF ₂	fluorspar F80	Cl ₂ H ₆ N ₂ Pt	cisplatin C350
CaH ₂ O ₂	calcium hydroxide C33	Cl ₂ MgO ₆	magnesium chlorate M3
CaH ₄ O ₆ S	calcium sulfate dihydrate C45	Cl ₂ MgO ₈	magnesium perchlorate M7
CaMn ₂ O ₈	calcium permanganate C38	Cl ₂ Ni	nickel chloride N46
CaN ₂ O ₆	calcium nitrate C36	Cl ₂ OS	thionyl chloride T136
CaO	calcium oxide C37	Cl ₂ OSe	selenium oxychloride S19
CaO ₂	calcium peroxide C39	Cl ₂ O ₈ Pb	lead perchlorate L26
CaO ₄ S ₂	calcium dithionite C31	Cl ₂ Pb	lead chloride L15
CaS	calcium sulfide C46	Cl ₂ Pd	palladium chloride P2
CaSO ₄	calcium sulfate C44	Cl ₂ Pt	platinum dichloride P213
CaSiO ₃	calcium silicate C43	Cl ₂ Sn	tin(II) chloride T159
Ca ₃ O ₈ P ₂	calcium phosphate C40	Cl ₂ S ₂	sulfur monochloride S154
Ca ₃ P ₂	calcium phosphide C41	Cl ₂ Zn	zinc chloride Z6
Cd	cadmium C2	Cl ₃ Cr	chromium(III) chloride C334
CdBr ₂	cadmium bromide C4	Cl ₃ Fe	iron(III) chloride I69
CdCl ₂	cadmium chloride C5	Cl ₃ HSi	trichlorosilane T267
CdF ₂	cadmium fluoride C7	Cl ₃ La	lanthanum trichloride L5
CdF ₆ Si	cadmium fluorosilicate C8	Cl ₃ OP	phosphorus oxychloride P159
CdI ₂	cadmium iodide C10	Cl ₃ OV	vanadium oxytrichloride V11
CdO	cadmium oxide C11	Cl ₃ P	phosphorus trichloride P166
CdO ₄ S	cadmium sulfate C13	Cl ₃ PS	thiophosphoryl chloride T141
CdS	cadmium sulfide C14	Cl ₃ Rh	rhodium trichloride R11
Ce	cerium C101	Cl ₃ Ti	titanium trichloride T167
ClCu	copper(I) chloride C433	Cl ₃ V	vanadium trichloride V14
ClCu ₂ H ₃ O ₃	copper oxychloride C441	Cl ₃ Y	yttrium chloride Y3
ClFO ₃	perchloryl fluoride P53	Cl ₄ Ir	iridium tetrachloride I65
ClF ₃	chlorine trifluoride C138	Cl ₄ Os	osmium tetrachloride O38
ClF ₅	chlorine pentafluoride C137	Cl ₄ Pt	platinum tetrachloride P214
ClHO ₃ S	chlorosulfonic acid C285	Cl ₄ Sn	tin(IV) chloride T160
ClHO ₄	perchloric acid P52	Cl ₄ Te	tellurium tetrachloride T18
ClH ₂ N	chloramine C112	Cl ₄ Th	thorium chloride T149
ClH ₄ N	ammonium chloride A169	Cl ₄ Ti	titanium tetrachloride T166
ClH ₁₀ O ₆ Na	sodium hypochlorite pentahydrate S75	Cl ₄ V	vanadium tetrachloride V13
ClI	iodine monochloride I41	Cl ₄ Zr	zirconium tetrachloride Z24
ClK	potassium chloride P243	Cl ₅ P	phosphorus pentachloride P160
ClKO ₃	potassium chlorate P242	Cl ₆ H ₂ Pt	chloroplatinic acid C261
ClKO ₄	potassium perchlorate P259	Cl ₆ H ₈ N ₂ Pt	ammonium chloroplatinate(IV) A170
ClLiO	lithium hypochlorite L55	Co	cobalt C369
ClNO	nitrosyl chloride N177	CoCl ₂	cobalt(II) chloride C372
ClNaO	sodium hypochlorite S74	CoH ₄ N ₂ O ₆ S ₂	cobalt(II) sulfamate C378
ClNaO ₂	sodium chlorite S54	CoO	cobalt(II) oxide C376
ClNaO ₃	sodium chlorate S53	CoO ₄ S	cobalt(II) sulfate C379
ClNaO ₄	sodium perchlorate S83	CoS	cobalt(II) sulfide C380
ClO ₂	chlorine dioxide C136	Cr	chromium C329
ClTI	thallium(I) chloride T103	Cr	chromium(III) C330

Cr	chromium(vi) C331	F ₆ Si	fluorosilicate F73
CrF ₃	chromium(III) fluoride C335	F ₆ SiPb	lead hexafluorosilicate L23
CrH ₂ O ₄	chromic acid C328	F ₆ Te	tellurium hexafluoride T17
CrH ₈ N ₂ O ₄	ammonium chromate A171	F ₆ W	tungsten hexafluoride T373
CrK ₂ O ₄	potassium chromate P244	F ₁₀ S ₂	disulfur decafluoride D568
CrN ₃ O ₉	chromium(III) nitrate C336	Fe	iron I66
CrNa ₂ O ₄	sodium chromate S56	FeF ₃	iron(III) fluoride I71
CrO ₃	chromium(vi) oxide C337	FeH ₈ N ₂ O ₈ S ₂	iron(II) ammonium sulfate I67
CrO ₄ Sr	strontium chromate S122	FeN ₃ O ₉	iron(III) nitrate I73
CrO ₄ Zn	zinc chromate Z7	FeO ₄ S	iron(II) sulfate I76
Cr ₂ H ₄ Na ₂ O ₉	sodium dichromate dihydrate S62	Fe ₂ O ₃	iron(III) oxide I74
Cr ₂ H ₈ N ₂ O ₇	ammonium dichromate A172	Fe ₂ O ₁₂ S ₃	iron(III) sulfate I77
Cr ₂ K ₂ O ₇	potassium dichromate P246	Fr	francium F110
Cr ₂ Na ₂ O ₇	sodium dichromate S61	Ga	gallium G3
Cr ₂ O ₁₂ S ₃	chromium(III) sulfate C338	GaAs	gallium arsenide G4
Cs	caesium C16	GaCl ₃	gallium trichloride G7
CsHO	caesium hydroxide C17	GaN ₃ O ₉	gallium nitrate G5
CsNO ₃	caesium nitrate C18	Ga ₂ O ₃	gallium oxide G6
Cu	copper C429	Gd	gadolinium G1
CuH ₁₂ N ₄ O ₄ S	copper sulfate, ammoniated C443	GeH ₄	germanium tetrahydride G13
CuN ₂ O ₆	copper nitrate C438	HBr	hydrogen bromide H98
CuO ₄ S	copper sulfate C442	HCl	hydrogen chloride H99
Cu ₂ O	copper(I) oxide C440	HF	hydrogen fluoride H101
D ₂	deuterium D61	HI	hydrogen iodide H102
Dy	dysprosium D604	HKO	potassium hydroxide P254
Eu	europium E189	HKO ₄ S	potassium hydrogen sulfate P253
FHO ₃ S	fluorosulfonic acid F75	HNO ₃	nitric acid N68
FH ₄ N	ammonium fluoride A173	HN ₃	hydrogen azide H97
FK	potassium fluoride P248	HN ₅	sodium hydride S70
FNa	sodium fluoride S66	HN ₅ O	sodium hydroxide S73
F ₂	fluorine F52	HNaO ₃ S	sodium bisulfite S48
F ₂ HK	potassium hydrogen fluoride P252	HNaS	sodium hydrosulfide S72
F ₂ HNa	sodium hydrogen fluoride S71	HNa ₂ O ₄ P	sodium monohydrogen phosphate S79
F ₂ H ₅ N	ammonium hydrogen difluoride A175		rubidium hydroxide R20
F ₂ O	oxygen difluoride O61	HORb	thallium hydrogen sulfate T104
F ₂ O ₂ S	sulfuryl fluoride S158	HO ₄ STl	hydrogen H96
F ₂ Pb	lead fluoride L22	H ₂	Bordeaux mixture B142
F ₂ Sn	tin(II) fluoride T161	H ₂ Ca ₃ Cu ₄ S ₂ O ₁₀	cadmium chloride monohydrate C6
F ₃ N	nitrogen trifluoride N121	H ₂ Cl ₂ OCd	fluorophosphoric acid F71
F ₄ S	sulfur tetrafluoride S156		talc T3
F ₅ P	phosphorus pentafluoride P161	H ₂ FO ₃ P	sodium amide S41
F ₅ Sb	antimony pentafluoride A224	H ₂ Mg ₃ O ₁₂ Si ₄	nickel hydroxide N47
F ₆ H ₂ Si	fluorosilicic acid F74	H ₂ NNa	hydrogen peroxide H103
F ₆ H ₈ N ₂ Si	ammonium fluorosilicate A174	H ₂ NiO ₂	sulfurous acid S155
F ₆ K ₂ Si	potassium fluorosilicate P250	H ₂ O ₂	selenious acid S13
F ₆ K ₂ Zr	potassium fluorozirconate(IV) P251	H ₂ O ₃ S	sulfuric acid S152
F ₆ MgSi	magnesium fluorosilicate M4	H ₂ O ₃ Se	selenic acid S12
F ₆ Na ₂ Si	sodium fluorosilicate S68	H ₂ O ₄ S	sulfuric acid (fuming) S153
F ₆ S	sulfur hexafluoride S151	H ₂ O ₄ Se	hydrogen sulfide H105
		H ₂ O ₇ S ₂	hydrogen selenide H104
		H ₂ S	
		H ₂ Se	

H ₂ Zr	zirconium hydride Z21	IKO ₃	potassium iodate P255
H ₃ NO	hydroxylamine H112	InP	indium phosphide I28
H ₃ NO ₃ S	sulfamic acid S137	I ₂	iodine I40
H ₃ O ₃ P	phosphorous acid P157	I ₂ Pb	lead iodide L24
H ₃ O ₄ P	phosphoric acid P156	Ir	iridium I64
H ₃ P	phosphine P155	K	potassium P237
H ₄ BF ₄ N	ammonium tetrafluoroborate A189	KMnO ₄	potassium permanganate P260
H ₄ NO ₃ V	ammonium metavanadate A177	KNO ₂	potassium nitrite P258
H ₄ N ₂	hydrazine H87	KNO ₃	potassium nitrate P257
H ₄ N ₂ O ₃	ammonium nitrate A178	KO ₂	potassium superoxide P265
H ₄ O ₁₁ P ₂ Pb ₆	lead phosphite dibasic L28	K ₂ O ₄ S	potassium sulfate P264
H ₄ Si	silane S28	K ₂ O ₈ S ₂	potassium persulfate P261
H ₅ NO	ammonium hydroxide A176	La	lanthanum L4
H ₅ NO ₃ S	ammonium bisulfite A166	Li	lithium L52
H ₆ N ₂ O	hydrazine hydrate H88	LiH	lithium hydride L54
H ₆ N ₂ O ₃ S	ammonium sulfamate A184	Lu	lutetium L60
H ₆ N ₂ O ₄ S	hydrazine sulfate H89	Mn	manganese M22
H ₈ N ₂ NiO ₈ S ₂	nickel ammonium sulfate N45	MnN ₂ O ₆	manganese nitrate M26
H ₈ N ₂ O ₃ S	ammonium sulfite A187	MnO ₂	manganese dioxide M24
H ₈ N ₂ O ₄ S	ammonium sulfate A185	Mn ₃ O ₄	manganese tetroxide M27
H ₈ N ₂ O ₈ S ₂	ammonium peroxydisulfate A181	MgN ₂ O ₆	magnesium nitrate M5
H ₈ N ₂ S	ammonium sulfide A186	MgO	magnesium oxide M6
H ₈ N ₂ S ₂ O ₃	ammonium thiosulfate A191	Mg ₃ P ₂	magnesium phosphide M8
H ₈ N ₂ S ₃	ammonium polysulfide A183	Mg ₃ Si ₂ O ₉ H ₄	chrysotile C342
H ₂₄ O ₁₆ Na ₃ P	trisodium phosphate dodecahydrate T360	Mo	molybdenum M338
He	helium H11	MoO ₃	molybdenum trioxide M339
Hf	hafnium H1	NH ₃	ammonia A161
HfCl ₄	hafnium chloride H2	NNaO ₂	sodium nitrite S81
Hg	mercury M64	NNaO ₃	sodium nitrate S80
HgBr ₂	mercury(II) bromide M69	NO	nitric oxide N69
HgCl	mercury(I) chloride M70	NO ₂	nitrogen dioxide N120
HgCl ₂	mercury(II) chloride M71	NO ₃ Tl	thallium(I) nitrate T106
HgI	mercury(I) iodide M75	N ₂	nitrogen N119
HgI ₂	mercury(II) iodide M76	N ₂ O	nitrous oxide N183
HgI ₄ K ₂	potassium tetraiodomercurate(II) P266	N ₂ O ₃	dinitrogen trioxide D479
HgNH ₂ Cl	mercury ammonium chloride M66	N ₂ O ₄	dinitrogen tetroxide D478
HgN ₂ O ₆	mercury(II) nitrate M78	N ₂ O ₅	dinitrogen pentoxide D477
HgO	mercury(II) oxide M82	N ₂ O ₆ Pb	lead nitrate L25
HgO ₄ S	mercury(II) sulfate M86	N ₂ O ₆ Sr	strontium nitrate S123
Hg ₂ Br ₂	mercury(I) bromide M68	N ₂ O ₆ Zn	zinc nitrate Z11
Hg ₂ Cl ₂	calomel C47	N ₂ O ₈ U	uranyl nitrate U11
Hg ₂ N ₂ O ₆	mercury(I) nitrate M77	N ₃ Na	sodium azide S47
Hg ₂ O	mercury(I) oxide M81	N ₃ O ₉ Y	yttrium nitrate Y4
Hg ₂ O ₄ S	mercury(I) sulfate M85	N ₄ O ₁₂ Th	thorium nitrate T151
Ho	holmium H83	N ₄ O ₁₂ Zr	zirconium nitrate Z22
In	indium I27	Na	sodium S39
InCl ₃	indium trichloride I29	Na ₂ FO ₃ P	disodium fluorophosphate D563
IK	potassium iodide P256	Na ₂ O ₃ S	sodium sulfite S94
		Na ₂ O ₃ Se	sodium selenite S90
		Na ₂ O ₃ Te	sodium tellurite S95
		Na ₂ O ₄ S	sodium sulfate S92
		Na ₂ O ₄ Se	sodium selenate S89

$\text{Na}_2\text{O}_4\text{W}$	sodium tungstate S99	PSr	strontium phosphide S124
$\text{Na}_2\text{O}_5\text{S}_2$	sodium metabisulfite S78	P_2S_5	phosphorus pentasulfide P162
$\text{Na}_2\text{O}_8\text{S}_2$	sodium persulfate S84	P_2Zn_3	zinc phosphide Z14
Na_2S	sodium sulfide S93	P_4S_3	phosphorus sesquisulfide P164
$\text{Na}_3\text{O}_4\text{P}$	trisodium phosphate T359	Pb	lead L11
Na_3P	sodium phosphide S87	PbCrO_4	lead chromate L16
$\text{Na}_4\text{O}_7\text{P}_2$	sodium pyrophosphate S88	PbS	lead sulfide L31
$\text{Na}_5\text{O}_{10}\text{P}_3$	sodium triphosphate S98	Pr	praseodymium P268
$\text{Na}_6\text{O}_{18}\text{P}_6$	sodium hexametaphosphate S69	Pt	platinum P212
Nb	niobium N61	Rn	radon R1
Nd	neodymium N33	Rb	rubidium R19
Ni	nickel N44	Re	rhodium R8
NiN_2O_6	nickel nitrate N48	Rh	rhodium R10
NiO_4S	nickel sulfate N50	Ru	ruthenium R21
Ni_3S_2	nickel subsulfide N49	S	sulfur S149
OZn	zinc oxide Z12	Sn	tin T158
O_2	oxygen O60	SSe	selenium sulfide S20
O_2Pb	lead dioxide L19	S_2Se	selenium disulfide S17
O_2S	sulfur dioxide S150	Sb	antimony A221
O_2Se	selenium dioxide S16	SbCl_3	antimony trichloride A225
O_2Si	silica S29	SbCl_5	antimony pentachloride A223
O_2Si	tridymite T274	SbF_3	antimony trifluoride A226
O_2Si	quartz Q1	Sb_2O_3	antimony trioxide A227
O_2Th	thorium dioxide T150	Se	selenium S14
O_2Ti	titanium dioxide T165	SeF_6	selenium hexafluoride S18
O_3	ozone O65	Si	silicon S30
O_3P_2	phosphorus trioxide P167	Sm	samarium S7
O_3S	sulfur trioxide S157	Sr	strontium S121
O_3Tl_2	thallium(III) oxide T107	Ta	tantalum T7
O_3V_2	vanadium trioxide V15	Tb	terbium T21
O_4Os	osmium tetroxide O39	Te	tellurium T16
O_4SPb	lead sulfate L30	Th	thorium T148
O_4STl_2	thallium(I) sulfate T108	Ti	titanium T164
O_4SZn	zinc sulfate Z17	Tl	thallium T100
O_5P_2	phosphorus pentoxide P163	U	uranium U9
O_5SV	vanadyl sulfate V16	V	vanadium V10
O_5V_2	vanadium pentoxide V12	W	tungsten T371
$\text{O}_8\text{P}_2\text{Pb}_3$	lead phosphate L27	Y	yttrium Y2
$\text{O}_8\text{S}_2\text{Zr}$	zirconium(IV) sulfate Z23	Zn	zinc Z2
Os	osmium O37	Zr	zirconium Z20
P	phosphorus P158		

ISBN 0-85404-838-3



9 780854 048380 >