Dictionary of Organic Compounds

SIXTH EDITION

FIRST SUPPLEMENT

Volume 10 of Dictionary of Organic Compounds

Springer-Science+ Business Media, B.V.

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First Supplement

1. Introduction

For detailed information about how to use the *Dictionary of Organic Compounds* (DOC) see the Introduction in Volume 1 of the Main Work.

1. Using DOC 6 Supplements

As in the Main Work volumes, every Entry is numbered to assist ready location. The DOC Number consists of a letter of the alphabet followed by a five-digit number. In this First Supplement the first digit is invariably 1. Cross-references within the text to Entries having numbers beginning with zero refer to Main Work Entries.

Where a Supplement Entry contains additional or corrected information referring to an Entry in the Main Work the whole Entry is reprinted, with the accompanying statement "Updated Entry replacing ...". In such cases, the new Entry contains all of the information which appeared in the former Entry, except for any which has been deliberately deleted. Therefore there is no necessity for the user to consult the Main Work or previous supplements.

2. Literature coverage

In compiling this Supplement the primary literature has been surveyed to the end of 1995. A considerable number of amendments have been made during the review period to entries which have not been reprinted in the Supplement owing to space limitations. All of these can be accessed via the CD-ROM version.

3. Indexes

The indexes in the Supplement consist of Name, Molecular Formula and CAS Registry Number Index.

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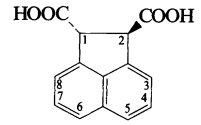
A

1,2-Acenaphthenedicarboxylic acid A-1-00001

Updated Entry replacing A-0-00042

1,2-Dihydro-1,2-acenaphthylenedicarboxylic acid, 9CI



(1*S*,2*S*)-*form*

$C_{14}H_{10}O_4$ M 242.2

(1S,2S)-form [51869-92-2]
(+)-trans-*form*
$[\alpha]_D^{25}$ +209 (EtOH).

Di-Me ester: [51869-93-3].
$C_{16}H_{14}O_4$ M 270.2 Cryst. (Et_2O). Mp 115.5°. $[\alpha]_D^{25}$ +179 (EtOH).

(1RS,2RS)-form [51869-91-1]
(±)-trans-*form*
Cryst. (C_6H_6/AcOH). Mp 234° dec.

Di-Me ester: [56137-60-1].
Cryst. (MeOH). Mp 85°.

(1RS,2SR)-form [5673-06-3]
cis-*form*
Cryst. (H_2O). Mp 179° dec.

Di-Me ester: [5673-22-3].
Mp 125°.

Anhydride:
$C_{14}H_8O_3$ M 224.2 Needles (C_6H_6). Mp 184°.

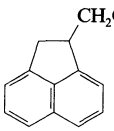
Canceill, J. *et al*, *Bull. Soc. Chim. Fr.*, 1974, 2833.

Parvez, M. *et al*, *Acta Cryst. C*, 1995, **51**, 644 (*cryst struct, abs config*)

1-Acenaphthenemethanol A-1-00002

1,2-Dihydro-1-acenaphthylenemethanol, 9CI. 1-(Hydroxymethyl)acenaphthene

[37977-49-4]

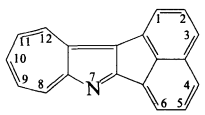


$C_{13}H_{12}O$ M 184.2

(±)-form
No phys. props. descr.

Haddad, N. *et al*, *J.O.C.*, 1994, **59**, 6090 (*synth, ir, pmr*)

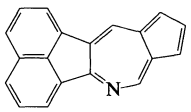
Acenaphtho[1,2-*b*]cyclohepta[*d*]pyrrole A-1-00003



$C_{19}H_{11}N$ M 253.3
Dark violet needles. Mp 196-197°. pK_a 5.6 (MeCN/aq. buffer).

Nitta, M. *et al*, *J.C.S. Perkin 1*, 1994, 2721 (*synth, uv, pmr, cmr*)

Acenaphtho[1,2-*b*]cyclopenta[*e*]azepine A-1-00004



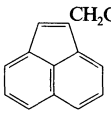
$C_{19}H_{11}N$ M 253.3
Green prisms (EtOH). Mp 170°.

Nitta, M. *et al*, *J.C.S. Perkin 1*, 1995, 1001 (*synth, pmr, cmr, ir*)

1-Acenaphthylenemethanol, 9CI A-1-00005

1-(Hydroxymethyl)acenaphthylene

[158779-89-6]



$C_{13}H_{10}O$ M 182.2
Cryst. Mp 49-50°.

Haddad, N. *et al*, *J.O.C.*, 1994, **59**, 6090 (*synth, ir, pmr, uv*)

(1-Acetoxyethenyl)phosphonic acid A-1-00006

(1-Acetoxyvinyl)phosphonic acid

[65864-85-9]

$H_2C{=}C(OAc)P(O)(OH)_2$

$C_4H_7O_5P$ M 166.0

Di-Me ester: [17674-23-6]. *Dimethyl (1-acetoxyethenyl)phosphonate*
$C_6H_{11}O_5P$ M 194.1 Liq. Bp_{18} 136°.

Di-Et ester: [17572-67-7]. *Diethyl (1-acetoxyethenyl)phosphonate*
$C_8H_{15}O_5P$ M 222.1 Liq. Bp_{18} 137°, $Bp_{0.06}$ 68°. n_D^{20} 1.4368.

Dipropyl ester: [17572-68-8]. *Dipropyl (1-acetoxyethenyl)phosphonate*
$C_{10}H_{19}O_5P$ M 250.2 Liq. $Bp_{0.1}$ 65°.

Diisopropyl ester: [40878-92-0]. *Diisopropyl (1-acetoxyethenyl)phosphonate*
$C_{10}H_{19}O_5P$ M 250.2 Liq. Bp_{16} 138°.

Dibutyl ester: [17474-70-3]. *Dibutyl (1-acetoxyethenyl)phosphonate*
$C_{12}H_{23}O_5P$ M 278.2 Liq. $Bp_{0.1}$ 72°.

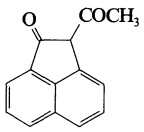
Dichloride: [144917-47-5].
$C_4H_5Cl_2O_3P$ M 202.9 Phys. props. not reported.

Al'fonsov, V.A. *et al*, *Zh. Obshch. Khim.*, 1984, **54**, 1485; *J. Gen. Chem. USSR (Engl. Transl.)*, 1984, **54**, 1324 (*synth, pmr, P-31 nmr*)

Tyryshkin, N.I. *et al*, *Heteroat. Chem.*, 1992, **3**, 127 (*esters, synth, ir, pmr, cmr, P-31 nmr*)

Shvedova, Yu.I. *et al*, *Zh. Obshch. Khim.*, 1992, **92**, 593; *J. Gen. Chem. USSR (Engl. Transl.)*, 1992, **62**, 486 (*dichloride, synth, pmr, P-31 nmr*)

2-Acetylacenaphthenone A-1-00007



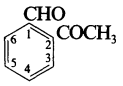
$C_{14}H_{10}O_2$ M 210.2
Yellow needles (hexane). Mp 118-119°.

Tsuge, O. *et al*, *J. Het. Chem.*, 1994, **31**, 1283.

2-Acetylbenzaldehyde, 9CI A-1-00008

2-Formylacetophenone

[24257-93-0]



$C_9H_8O_2$ M 148.1
Needles (pentane). Mp 44° (41-42°).

Bis(2,4-dinitrophenylhydrazone): [24257-94-1]. Mp 137-140°.

Berner, E., *Acta Chem. Scand., Ser. B*, 1982, **36**, 729 (*synth*)

Sternson, L.A. *et al*, *Anal. Biochem.*, 1985, **144**, 233 (*synth, pmr, ms*)

Moriarty, R.M. *et al*, *Synthesis*, 1993, 318 (*synth, pmr, cmr*)

3-Acetylbenzaldehyde, 9CI A-1-00009

3-Formylacetophenone

[41908-11-6]

$C_9H_8O_2$ M 148.1
Cryst. (hexane). Mp 49.5-51° (42-45°). Bp_{15} 147-151°.

Dioxime:
$C_9H_{10}N_2O_2$ M 178.1 Mp 124.5-126°.

Bisphenylhydrazone: [61494-01-7]. Mp 163-166°.

Karmanova, I.B. *et al*, *Khim. Geterotsikl. Soedin.*, 1973, 490; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1973, 451 (*synth*)

Tinapp, P. *et al*, *Arch. Pharm. (Weinheim, Ger.)*, 1976, **309**, 766 (*synth*)

4-Acetylbenzaldehyde, 9CI A-1-00010

4-Formylacetophenone

[3457-45-2]

$C_9H_8O_2$ M 148.1
Cryst. Mp 34°. Bp_{15} 152-155°.

Dioxime:
$C_9H_{10}N_2O_2$ M 178.1 Needles. Mp 180.6-181.2°.

Bisphenylhydrazone: Yellow needles (EtOH). Mp 189.6-190.8°.

Detweiler, W.K. *et al*, *J.A.C.S.*, 1950, **72**, 2882 (*synth, derivs*)

Stille, J.K. *et al*, *J.O.C.*, 1979, **44**, 1613 (*synth, pmr*)

Kauffmann, T. *et al*, *Chem. Ber.*, 1992, **125**, 899 (*synth*)

N-Acetyl-*N'*-benzoylhydrazine A-1-00011

Benzoic acid 2-acetylhydrazide, 9CI

[14331-27-2]

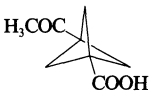
PhCONHNHAc

$C_9H_{10}N_2O_2$ M 178.1
Cryst. (H_2O). Mp 175-176°.

Horwitz, J.P. *et al, J.O.C.*, 1954, **19**, 194 (*synth, bibl*)
Carlsen, P.H.J. *et al, J. Het. Chem.*, 1994, **31**, 805 (*synth, pmr, cmr, ir*)

3-Acetylbicyclo[1.1.1]pentane-1-carboxylic acid, 9CI A-1-00012

[156329-75-8]



$C_8H_{10}O_3$ M 154.1
Cryst. by subl. Mp 95-96°.

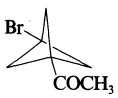
Me ester: [131515-42-9].
$C_9H_{12}O_3$ M 168.1 Cryst. Mp 59-59.5°.

Kaszynski, P. *et al, J.O.C.*, 1991, **56**, 307 (*Me ester, synth, pmr, cmr, ir, ms*)
Della, E.W. *et al, J.O.C.*, 1994, **59**, 2986 (*synth, ir, pmr, cmr, ms*)

1-Acetyl-3-bromobicyclo[1.1.1]pentane A-1-00013

1-(3-Bromobicyclo[1.1.1]pent-1-yl)ethanone, 9CI

[156329-63-4]



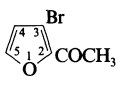
C_7H_9BrO M 189.0
Cryst. Mp 43.5-44°.

Della, E.W. *et al, J.O.C.*, 1994, **59**, 2986 (*synth, ir, pmr, cmr, ms*)

2-Acetyl-3-bromofuran A-1-00014

1-(3-Bromo-2-furanyl)ethanone, 9CI. 3-Bromo-2-furyl methyl ketone, 8CI

[22037-29-2]



$C_6H_5BrO_2$ M 189.0
Cryst. (Et_2O/hexane) or needles ($CHCl_3$/hexane). Mp 45°. Bp_{20} 110-114°.

Semicarbazone: [22037-30-5]. Mp 221-222°.

Nazarova, Z.N. *et al, Khim. Geterotsikl. Soedin.*, 1969, 17; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1969, 12 (*synth*)
Zaluski, M.-C. *et al, Bull. Soc. Chim. Fr.*, 1970, 1838 (*synth, pmr, ir*)
Gol'dfarb, Y.L. *et al, Khim. Geterotsikl. Soedin.*, 1970, 132; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1970, 129 (*synth*)
Koyanagi, J. *et al, J. Het. Chem.*, 1995, **32**, 1289 (*synth, ir, pmr, ms*)

2-Acetyl-4-bromofuran A-1-00015

1-(4-Bromo-2-furanyl)ethanone, 9CI

[3455-86-5]

$C_6H_5BrO_2$ M 189.0
Cryst. (EtOH aq.). Mp 69.5-70.5°.

Semicarbazone: Cryst. (EtOH). Mp 189-190°.

Gol'dfarb, Y.L. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1965, **163**, 1393; *Dokl. Chem. (Engl. Transl.)*, 1965, **163**, 805 (*synth*)
Belen'kii, L.I. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1973, **22**, 2666 (*pmr*)
Antonioletti, R. *et al, J.C.S. Perkin 1*, 1985, 1285 (*synth*)

2-Acetyl-5-bromofuran A-1-00016

1-(5-Bromo-2-furanyl)ethanone, 9CI. 5-Bromo-2-furyl methyl ketone

[3199-50-6]

$C_6H_5BrO_2$ M 189.0
Cryst. (heptane). Mp 92-94°.

Oxime:
$C_6H_6BrNO_2$ M 204.0 Cryst. (EtOH aq.). Mp 79.5°.

2,4-Dinitrophenylhydrazone: Red cryst. Mp 246-248°.

Gilman, H. *et al, J.A.C.S.*, 1931, **53**, 4193 (*synth, oxime*)
Vereshchagin, L.I. *et al, Zh. Org. Khim.*, 1965, **1**, 960; *J. Org. Chem. USSR (Engl. Transl.)*, 1965, **1**, 967 (*synth*)
Belen'kii, L.I. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1973, **22**, 2666 (*synth, pmr*)
Aly, S.A., *Indian J. Chem., Sect. B*, 1993, **32**, 566 (*synth*)

3-Acetyl-5-bromofuran A-1-00017

1-(5-Bromo-3-furanyl)ethanone, 9CI

[59227-68-8]

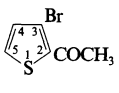
$C_6H_5BrO_2$ M 189.0
Cryst. or cream solid. Mp 68-70°.

Roques, B.-P. *et al, Bull. Soc. Chim. Fr.*, 1975, 2334 (*synth*)
Eur. Pat., 399 645, (1990); *CA*, **114**, 228892a (*synth, pmr*)

2-Acetyl-3-bromothiophene A-1-00018

1-(3-Bromo-2-thienyl)ethanone, 9CI. 3-Bromo-2-thienyl methyl ketone

[42877-08-7]



C_6H_5BrOS M 205.0
Pale green liq. Bp_4 104°. n_D^{20} 1.6108.

Oxime, (E)-: [98453-19-1].
C_6H_6BrNOS M 220.0 Cryst. (heptane). Mp 111-112°.

Gol'dfarb, Y.L. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1959, **128**, 536; *Dokl. Chem. (Engl. Transl.)*, 1959, **128**, 767 (*synth*)
Conde, S. *et al, J. Het. Chem.*, 1985, **22**, 301 (*oxime*)
Greiner-Bechert, L. *et al, Arch. Pharm. (Weinheim, Ger.)*, 1991, **324**, 563 (*synth, pmr, cmr*)

2-Acetyl-4-bromothiophene A-1-00019

1-(4-Bromo-2-thienyl)ethanone, 9CI. 4-Bromo-2-thienyl methyl ketone, 8CI

[7209-11-2]

C_6H_5BrOS M 205.0
Liq. Bp_{15} 133-135°. n_D^{20} 1.6080.

Oxime, (E)-: [98453-20-4].
C_6H_6BrNOS M 220.0 Mp 152-154°.

Oxime, (Z)-: [98453-22-6].
C_6H_6BrNOS M 220.0 Mp 143-145°.

Semicarbazone: [33148-62-8]. Mp 214.5-215°.

Gol'dfarb, Y.L. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1959, **128**, 536; *Dokl. Chem. (Engl. Transl.)*, 1959, **128**, 767 (*synth*)
Vol'kenshtein, Y.B. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1961, 1879; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1961, 1752 (*synth, uv, ir*)
Alvarez-Insúa, A.S. *et al, J. Het. Chem.*, 1982, **19**, 713 (*synth, pmr*)
Conde, S. *et al, J. Het. Chem.*, 1985, **22**, 301 (*oximes*)

3-Acetyl-4-bromothiophene A-1-00020

1-(4-Bromo-3-thienyl)ethanone, 9CI

[35717-24-9]

C_6H_5BrOS M 205.0
Liq. Bp_{12} 137°.

Spinelli, D. *et al, J.C.S. Perkin 2*, 1972, 441 (*synth*)
Hanquet, B. *et al, Bull. Soc. Chim. Fr.*, 1977, 571 (*synth, pmr*)
Juliá, S. *et al, Afinidad*, 1984, **41**, 145; *CA*, **101**, 90700j (*synth, ir, uv, pmr, ms*)

3-Acetyl-5-bromothiophene A-1-00021

1-(5-Bromo-3-thienyl)ethanone, 9CI

[59227-67-7]

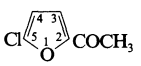
C_6H_5BrOS M 205.0
Cryst. Mp 63-64°. Bp_{13} 130-135°.

Roques, B.-P. *et al, Bull. Soc. Chim. Fr.*, 1975, 2334 (*synth*)
Karlsson, O., *Synth. Commun.*, 1981, **11**, 29 (*synth*)

2-Acetyl-5-chlorofuran A-1-00022

1-(5-Chloro-2-furanyl)ethanone, 9CI

[3216-65-7]



$C_6H_5ClO_2$ M 144.5
Cryst. Mp 79°.

Semicarbazone: Mp 196-197°.

Nazarova, Z.N. *et al, Zh. Obshch. Khim.*, 1963, **33**, 1431; *J. Gen. Chem. USSR (Engl. Transl.)*, 1963, **33**, 1397 (*synth*)
D'Auria, M. *et al, Synthesis*, 1995, 248 (*synth*)

3-Acetyl-5-chlorofuran A-1-00023

1-(5-Chloro-3-furanyl)ethanone, 9CI

[59227-69-9]

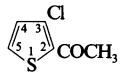
$C_6H_5ClO_2$ M 144.5
Cryst. Mp 51°.

Roques, B.-P. *et al, Bull. Soc. Chim. Fr.*, 1975, 2334 (*synth*)

2-Acetyl-3-chlorothiophene A-1-00024

1-(3-Chloro-2-thienyl)ethanone, 9CI

[89581-82-8]



C_6H_5ClOS M 160.6
Liq. Bp_{15} 117-118°.

Profft, E. *et al, J. Prakt. Chem.*, 1964, **24**, 38 (*synth*)
Greiner-Bechert, L. *et al, Arch. Pharm. (Weinheim, Ger.)*, 1991, **324**, 563 (*synth, pmr*)

2-Acetyl-4-chlorothiophene A-1-00025

1-(4-Chloro-2-thienyl)ethanone, 9CI

[34730-20-6]

C_6H_5ClOS M 160.6
Liq. Bp_{10} 109-110°.

Juliá, S. *et al, Afinidad*, 1984, **41**, 145; *CA*, **101**, 90700j (*synth, ir, uv, pmr, ms*)
Stanetty, P. *et al, Monatsh. Chem.*, 1989, **120**, 53 (*synth, pmr*)

2-Acetyl-5-chlorothiophene A-1-00026

1-(5-Chloro-2-thienyl)ethanone, 9CI

[6310-09-4]

C_6H_5ClOS M 160.6
Cryst. (EtOH). Mp 52° (46°). Bp_{12} 104-106°.
Semicarbazone: Mp 233-234°.

Gattermann, L. *et al, Ber.*, 1886, **19**, 688 (*synth*)
Hartough, H.D. *et al, J.A.C.S.*, 1947, **69**, 1015 (*synth*)
Szmant, H.H. *et al, J.A.C.S.*, 1951, **73**, 4521 (*synth, uv*)
Kooreman, H.J. *et al, Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1967, **86**, 37 (*synth*)
D'Auria, M. *et al, Synthesis*, 1995, 248 (*synth*)

3-Acetyl-4-chlorothiophene A-1-00027

1-(4-Chloro-3-thienyl)ethanone, 9CI

[91387-31-4]

C_6H_5ClOS M 160.6
Liq. Bp_{20} 110-111°.

Juliá, S. *et al, Afinidad*, 1984, **41**, 145; *CA*, **101**, 90700j (*synth, ir, uv, pmr, ms*)

3-Acetyl-5-chlorothiophene A-1-00028

1-(5-Chloro-3-thienyl)ethanone, 9CI

[58119-67-8]

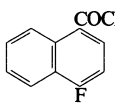
C_6H_5ClOS M 160.6
Cryst. Mp 57-58.5°. Bp_{10} 108-111°.

Hromatka, O. *et al, Monatsh. Chem.*, 1975, **106**, 1103 (*synth*)
Stanetty, P. *et al, Monatsh. Chem.*, 1989, **120**, 53 (*synth, pmr*)

1-Acetyl-4-fluoronaphthalene A-1-00029

1-(4-Fluoro-1-naphthalenyl)ethanone, 9CI. 4'-Fluoro-1'-acetonaphthone, 8CI

[316-68-7]



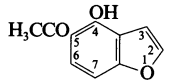
$C_{12}H_9FO$ M 188.2
Cryst. (hexane). d 1.20. Mp 38-39°. Bp_{17} 167°.
Oxime: [1717-24-4].
$C_{12}H_{10}FNO$ M 203.2 Needles (EtOH aq.). Mp 123-124°.

Jacobs, T.L. *et al, J.O.C.*, 1946, **11**, 27 (*synth*)
Adcock, W. *et al, J.A.C.S.*, 1976, **98**, 1701 (*oxime*)
Dixon, E.A. *et al, Can. J. Chem.*, 1981, **59**, 2629 (*synth*)

5-Acetyl-4-hydroxybenzofuran A-1-00030

1-(4-Hydroxy-5-benzofuranyl)ethanone, 9CI. 4-Hydroxy-5-benzofuranyl methyl ketone, 8CI

[69722-46-9]



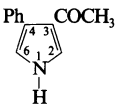
$C_{10}H_8O_3$ M 176.1
Degradation product of furanoflavones and furanochalcones. Pale yellow needles (MeOH aq.). Mp 95°.
Me ether: [52055-86-4]. *5-Acetyl-4-methoxybenzofuran*
$C_{11}H_{10}O_3$ M 190.1 Cryst. (hexane). Mp 54-55°.

Khanna, R.N. *et al, Tetrahedron*, 1963, **19**, 219.
Lee, Y.R. *et al, Tetrahedron*, 1995, **51**, 4909 (*synth, ir, pmr, cmr, ms*)

3-Acetyl-4-phenylpyrrole A-1-00031

1-(4-Phenyl-1H-pyrrol-3-yl)ethanone, 9CI

[40167-28-0]



$C_{12}H_{11}NO$ M 185.2
Cryst. (CH_2Cl_2/petrol). Mp 157-158°.

v. Leusen, A.M. *et al, Tet. Lett.*, 1972, 5337 (*synth*)
v. Leusen, D. *et al, J.O.C.*, 1992, **57**, 2245 (*synth, ir, pmr*)

4-Acetyl-2-phenylpyrrole A-1-00032

1-(5-Phenyl-1H-pyrrol-3-yl)ethanone, 9CI

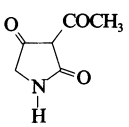
[148403-22-9]

$C_{12}H_{11}NO$ M 185.2
Cryst. (DMF aq.). Mp 176-178°.

Oda, K. *et al, Chem. Comm.*, 1993, 437 (*synth*)
Di Santo, R. *et al, Synth. Commun.*, 1995, **25**, 795 (*synth*)

3-Acetyl-2,4-pyrrolidinedione, 9CI A-1-00033

[697-57-4]

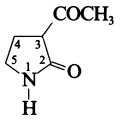


$C_6H_7NO_3$ M 141.1
Enolised β-diketone. Solid. Mp 174-176°.

Jones, R.C.F. *et al, J.C.S. Perkin 1*, 1994, 2513.

3-Acetyl-2-pyrrolidinone, 9CI A-1-00034

[31536-38-6]



$C_6H_9NO_2$ M 127.1
Prob. an enolised β-diketone. Prisms (hexane). Mp 77-78°.
N-*Me:* [60044-08-8].
$C_7H_{11}NO_2$ M 141.1 Bp_2 115-120°.

Kamenati, T. *et al, J.C.S.(C)*, 1971, 999 (*synth, pmr, ir*)

5-Acetyl-2-pyrrolidinone, 9CI A-1-00035

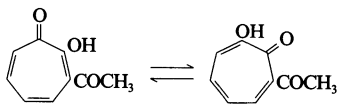
$C_6H_9NO_2$ M 127.1
(±)-***form*** [85858-09-9]
Cryst. (EtOAc). Mp 74-76°.

Thomas, E.J. *et al, J.C.S. Perkin 1*, 1983, 395 (*synth, ir, pmr*)

3-Acetyltropolone A-1-00036

3-Acetyl-2-hydroxy-2,4,6-cycloheptatrien-1-one, 9CI. 6-Acetyltropolone

[72023-82-6]

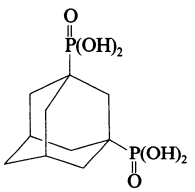


$C_9H_8O_3$ M 164.1
Pale yellow needles (MeOH). Mp 131-132°.

Yamane, A. *et al, Bull. Chem. Soc. Jpn.*, 1979, **52**, 1972 (*synth, uv, pmr*)

1,3-Adamantanediphosphonic acid A-1-00037

Tricyclo[3.3.1.1^{3,7}]decane-1,3-diylbisphosphonic acid, 9CI. 1,3-Adamantyldiphosphonic acid



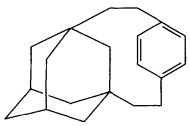
$C_{10}H_{18}O_6P_2$ M 296.1
Bis(diethyl) ester: [145290-43-3]. *Tetraethyl 1,3-adamantyldiphosphonate*
$C_{18}H_{34}O_6P_2$ M 408.4 Liq. $Bp_{0.01}$ 120°.
Bis(dichloride): [82316-74-3].
$C_{10}H_{14}Cl_4O_2P_2$ M 369.9 Cryst. Mp 171-173°.
Bis(dibromide):
$C_{10}H_{14}Br_4O_2P_2$ M 547.7 Cryst. Mp 222-224°.

Duddeck, H. *et al, Magn. Reson. Chem.*, 1985, **23**, 41, 533 (*cmr, O-17 nmr, P-31 nmr*)
Duddeck, H. *et al, Phosphorus Sulfur Relat. Elem.*, 1986, **28**, 307 (*synth, ir, ms, pmr*)
Petrov, K.A. *et al, Zh. Obshch. Khim.*, 1992, **62**, 303; *J. Gen. Chem. USSR (Engl. Transl.)*, 1992, **62**, 245 (*ester, ir, pmr*)

[2.2](1,3) Adamantanoparacyclophane A-1-00038

Pentacyclo[11.2.2.1^{4,8}.1^{4,10}.1^{6,10}]eicosa-13,15,16-triene, 9CI

[151133-06-1]



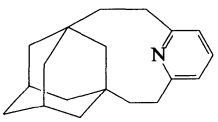
$C_{20}H_{26}$ M 266.4
Highly deformed mol. Cryst. Mp 95°.

Lemmerz, R. *et al, Chem. Comm.*, 1993, 1168 (*synth, pmr, cryst struct*)

[2.2](1,3)Adamantano-2,6-pyridinophane A-1-00039

20-Azapentacyclo[9.5.1.1^{1,13}.1^{4,8}.1^{11,15}]eicosa-4,6,8α(20)-triene, 9CI

[151133-07-2]



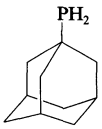
$C_{19}H_{25}N$ M 267.4
Cryst. Mp 89°.

Lemmerz, R. *et al, Chem. Comm.*, 1993, 1168 (*synth, pmr, cryst struct*)

1-Adamantylphosphine, 8CI A-1-00040

Tricyclo[3.3.1.1^{3,7}]dec-1-ylphosphine. 1-Phosphinoadamantane

[23906-89-0]



$C_{10}H_{17}P$ M 168.2
Liq. Bp_1 72°.

Oxide: [157426-62-5].
$C_{10}H_{17}OP$ M 184.2 Cryst. (EtOH). Mp 66°.

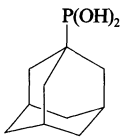
Sulfide: [87514-51-0].
$C_{10}H_{17}PS$ M 200.2 Cryst. (MeOH or EtOH). Mp 48°, Mp 82-84°.

Selenide: [87514-52-1].
$C_{10}H_{17}PSe$ M 247.1 Cryst. (MeOH or EtOH). Mp 84°, Mp 105-107°.

Stetter, H. *et al, Chem. Ber.*, 1969, **102**, 3364 (*synth*)
Zhardin, A.P. *et al, Zh. Obshch. Khim.*, 1983, **53**, 1429; *J. Gen. Chem. USSR (Engl. Transl.)*, 1983, **53**, 1285 (*synth, derivs, ir*)
Gouygou, M. *et al, Synthesis*, 1987, 508.
Yurchenko, R.I. *et al, Zh. Obshch. Khim.*, 1989, **59**, 2004; *J. Gen. Chem. USSR (Engl. Transl.)*, 1989, **59**, 1796 (*pmr*)
Goerlich, J.R. *et al, Z. Anorg. Allg. Chem.*, 1994, **620**, 898 (*synth, ms, pmr, P-31 nmr, complexes*)

1-Adamantylphosphonous acid A-1-00041

Tricyclo[3.3.1.1^{3,7}]dec-1-ylphosphonous acid. 1-Adamantanephosphonous acid



$C_{10}H_{17}O_2P$ M 200.2

Difluoride: [63429-85-6].
$C_{10}H_{15}F_2P$ M 204.1 Liq. $Bp_{0.04}$ 29.5°.

Dichloride: see *1-Adamantylphosphonous dichloride, A-0-00662*

Dibromide: [95927-88-1].
$C_{10}H_{15}Br_2P$ M 326.0 Solid. Mp 80-82°. Easily hydrol.

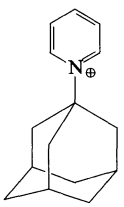
Diiodide: [141793-26-2].
$C_{10}H_{15}I_2P$ M 420.0 Cryst. (CH_2Cl_2/petrol or dioxan). Mp 42°, Mp 70-72°.

Uurchenko, R.I. *et al, Zh. Obshch. Khim.*, 1984, **54**, 2650; *J. Gen. Chem. USSR (Engl. Transl.)*, 1984, **54**, 2366 (*synth, P-31 nmr*)
Goerlich, J.R. *et al, Phosphorus, Sulfur, Silicon Relat. Elem.*, 1992, **66**, 223 (*dihalides, synth, ms, pmr, cmr, F-19 nmr, P-31 nmr*)

1-(1-Adamantyl)pyridinium(1+) A-1-00042

1-Tricyclo[3.3.1.1^{3,7}]dec-1-ylpyridinium, 9CI

[93588-28-4]



$C_{15}H_{20}N^{\oplus}$ M 214.3 (ion)

Bromide: [19984-57-7].
$C_{15}H_{20}BrN$ M 294.2 Mp 245° dec.

Perchlorate: [93588-29-5].
$C_{15}H_{20}ClNO_4$ M 313.7 Cryst. (EtOH).

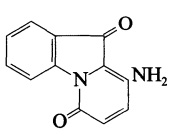
[112671-75-7]

U.S. Pat., 3 391 142, (1968); *CA*, **69**, 59281 (*synth*)
Katritzky, A.R. *et al, J. Chem. Res., Synop.*, 1984, 234 (*synth, pmr, cmr*)
Sokolenko, V.A. *et al, Khim. Geterotsikl. Soedin.*, 1987, 817 (*synth*)

Ailanindole A-1-00043

9-Aminopyrido[1,2-a]indole-6,10-dione, 9CI

[159903-51-2]

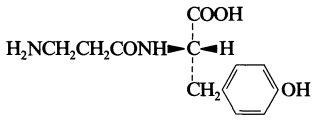


$C_{12}H_8N_2O_2$ M 212.2
Alkaloid from the wood of *Ailanthus malabarica* (Simaroubaceae). Orange needles (MeOH). Mp >300°. Intense green fluorescence in org. solvs.

Aono, H. *et al, Phytochemistry*, 1994, **37**, 579 (*isol, uv, ir, pmr, cmr, ms, struct*)

N-β-Alanyltyrosine A-1-00044

Sarcophagine†



$C_{12}H_{16}N_2O_4$ M 252.2

(S)-form [21612-26-0]

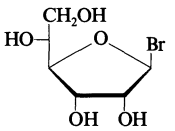
L-form
Isol. from the leaves of *Sarcophaga bullata* and *Phryxe caudata*. Mp 226-228°. $[\alpha]_D$ +43.5 (H_2O).

Z-β-Ala-Tyr-OH: [21612-25-9].
Cryst. (EtOAc/petrol). Mp 130-131°. $[\alpha]_D$ +16.2 (EtOH).

Z-β-Ala-Tyr-OMe: [21612-24-8].
Cryst. (EtOH/Et_2O/petrol). Mp 113-114°. $[\alpha]_D^{22}$ +5.9 (EtOH).

Pinelli, C. *et al, Farmaco, Ed. Sci.*, 1968, **23**, 859 (*synth*)
Levenbook, L. *et al, Biochem. J.*, 1969, **113**, 837 (*isol, synth*)
Bodnaryk, R.P., *Comp. Biochem. Physiol., B: Comp. Biochem.*, 1972, **43**, 587 (*isol*)

Allofuranosyl bromide A-1-00045



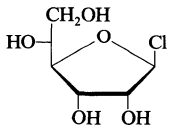
$C_6H_{11}BrO_5$ M 243.0

β-D-form

2,3:5,6-Di-O-isopropylidene: [65502-92-3].
$C_{12}H_{19}BrO_5$ M 323.1 Syrup.

Eitelman, S.J.E. *et al, Chem. Comm.*, 1977, 552 (*diisopropylidene, cmr*)
Eitelman, S.J.E. *et al, J.C.S. Perkin 1*, 1978, 595 (*diisopropylidene, pmr*)

Allofuranosyl chloride A-1-00046



β-D-*form*

$C_6H_{11}ClO_5$ M 198.6

D-form

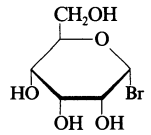
2,3:5,6-Di-O-isopropylidene: [33823-06-2].
$C_{12}H_{19}ClO_5$ M 278.7 Cryst. Mp 39-42°. $Bp_{0.1}$ 75-76°. Unstable at ambient temp.

β-D-form

2,3:5,6-Di-O-isopropylidene: [67253-98-9].
Oil. Not clear if this is the same as the D-diisopropylidene deriv.

Kohn, B.D. *et al, Carbohydr. Res.*, 1971, **18**, 349 (D-deriv)
Boigegrain, R.A. *et al, J. Chem. Res., Synop.*, 1978, 85; *J. Chem. Res., Miniprint*, 1978, 1229 (β-D-deriv)
Eitelman, S.J. *et al, J.C.S. Perkin 1*, 1978, 595 (β-D-deriv)
Bischofberger, K. *et al, S. Afr. J. Chem.*, 1981, **34**, 33 (β-D-deriv)

Allopyranosyl bromide A-1-00047



α-D-*form*

$C_6H_{11}BrO_5$ M 243.0

α-D-form

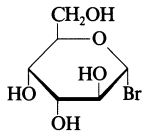
Tetra-Ac: [53369-42-9].
$C_{14}H_{19}BrO_9$ M 411.2 Pale yellow syrup. $[\alpha]_D^{23}$ +170.7 (c, 4.8 in $CHCl_3$).

β-D-form

Tetra-Ac: [75247-30-2].
Syrup.

Haga, M. *et al*, *Carbohydr. Res.*, 1974, **34**, 214 (*α-tetra-Ac, pmr*)
Stowell, C.P. *et al*, *Biochemistry*, 1980, **19**, 4899 (*β-tetra-Ac*)
Markham, K.R. *et al*, *Phytochemistry*, 1983, **22**, 2827 (*α-tetra-Ac, pmr*)
Cano, F.H. *et al*, *Carbohydr. Res.*, 1986, **145**, 319 (*α-tetra-Ac*)

Altropyranosyl bromide A-1-00048



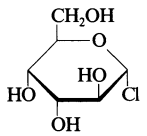
$C_6H_{11}BrO_5$ M 243.0

α-D-form

Tetra-Ac: [29907-26-4].
$C_{14}H_{19}BrO_9$ M 411.2 Cryst. Mp 107-108°. $[\alpha]_D^{20}$ +160 (c, 2.2 in $CHCl_3$).

de Pascual, J. *et al*, *An. Quim., Ser. B*, 1967, **63**, 221; *CA*, **67**, 82333f (*tetra-Ac*)
Paulsen, H. *et al*, *Chem. Ber.*, 1970, **103**, 2463; 1973, **106**, 3850 (*tetra-Ac*)

Altropyranosyl chloride A-1-00049



$C_6H_{11}ClO_5$ M 198.6

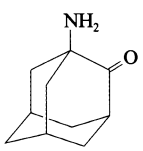
α-D-form

Tetra-Ac: [17081-03-7].
$C_{14}H_{19}ClO_9$ M 366.7 Cryst. ($CHCl_3$/Et_2O/2-methylbutane). Mp 102°. $[\alpha]_D^{20}$ +110 (c, 5 in $CHCl_3$).

Richtmyer, N.K. *et al*, *J.A.C.S.*, 1941, **63**, 1727 (*tetra-Ac*)
de Pascual, J. *et al*, *An. Quim., Ser. B*, 1967, **63**, 221; *CA*, **67**, 82333f (*tetra-Ac*)

1-Amino-2-adamantanone A-1-00050

1-Aminotricyclo[3.3.1.1^{3,7}]decanone, 9CI

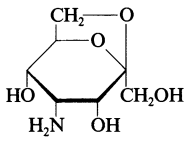


$C_{10}H_{15}NO$ M 165.2

Hydrochloride: [73228-03-2].
Solid. Mp 270-280° dec.

Sasaki, T. *et al*, *Synthesis*, 1980, 472 (*synth, ir, pmr*)

4-Amino-2,7-anhydro-4-deoxy-*allo*-heptulose A-1-00051



$C_7H_{13}NO_5$ M 191.1

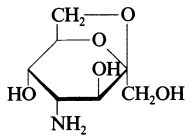
β-D-Pyranose-form

Prismatic columns (AcOH aq.) (as hydrochloride). $[\alpha]_D^{23}$ −54.7 (c, 1 in H_2O) (hydrochloride).

1,3,4N,5-Tetra-Ac:
$C_{15}H_{21}NO_9$ M 359.3 Platelets ($CHCl_3$/Et_2O). Mp 213-214° dec. $[\alpha]_D^{22}$ −60.9 (c, 1 in $CHCl_3$).

Baer, H.H. *et al*, *J.O.C.*, 1963, **28**, 1287; 1964, **29**, 2014 (*synth, tetra-Ac, pmr*)

4-Amino-2,7-anhydro-4-deoxy-*altro*-heptulose A-1-00052



$C_7H_{13}NO_5$ M 191.1

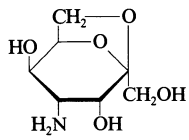
β-D-Pyranose-form

Needles (AcOH aq.) (as hydrochloride). $[\alpha]_D^{23}$ −126 (c, 1 in H_2O).

1,3,4N,5-Tetra-Ac:
$C_{15}H_{21}NO_9$ M 359.3 Needles ($CHCl_3$/Et_2O). Mp 189-190°. $[\alpha]_D^{22}$ −145.5 (c, 1 in $CHCl_3$).

Baer, H.H. *et al*, *J.O.C.*, 1963, **28**, 1287; 1964, **29**, 2014 (*synth, tetra-Ac, pmr*)

4-Amino-2,7-anhydro-4-deoxy-*gulo*-heptulose A-1-00053



$C_7H_{13}NO_5$ M 191.1

β-D-Pyranose-form

Prisms (AcOH aq.) (as hydrochloride). $[\alpha]_D^{23}$ +39 (c, 1 in H_2O).

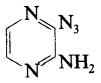
1,3,4N,5-Tetra-Ac:
$C_{15}H_{21}NO_9$ M 359.3 Prisms ($CHCl_3$/Et_2O). Mp 128-129°. $[\alpha]_D^{22}$ +43.7 (c, 1 in $CHCl_3$).

Baer, H.H. *et al*, *J.O.C.*, 1963, **28**, 1287; 1964, **29**, 2014 (*synth, tetra-Ac, pmr*)

2-Amino-3-azidopyrazine A-1-00054

3-Azido-2-pyrazinamine

[156331-25-8]

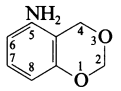


$C_4H_4N_6$ M 136.1
Microcryst. (EtOH). Mp 225° dec.

Sato, N. *et al*, *J.C.S. Perkin 1*, 1994, 885.

5-Amino-4*H*-1,3-benzodioxin A-1-00055

4H-1,3-Benzodioxin-5-amine, 9CI



$C_8H_9NO_2$ M 151.1
Mp 71-72°.

Hydrochloride: [52463-13-5].
Mp >280°.

N-*Ac:*
$C_{10}H_{11}NO_3$ M 193.2 Cryst. Mp 154-155°.

N,N-*Di-Me:* [52463-17-9].
$C_{10}H_{13}NO_2$ M 179.2 Liq.

N,N-*Di-Me; hydrochloride:* [52463-18-0].
Cryst. Mp 182°.

N,N,N-*Tri-Me:* [52463-22-6].
$C_{11}H_{16}NO_2^{\oplus}$ M 194.2 (ion) Cryst. (as chloride). Mp 202-203° dec.

[52463-20-4, 52463-21-5]

Ando, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1974, **47**, 501 (*synth, deriv*)

3-Amino-2-benzo[*b*]furancarboxaldehyde A-1-00056

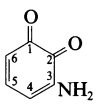
3-Amino-2-formylbenzo[b]*furan*

$C_9H_7NO_2$ M 161.1

Capperucci, A. *et al*, *J.O.C.*, 1995, **60**, 2254 (*synth, ir, pmr, cmr, ms*)

3-Amino-1,2-benzoquinone A-1-00057

3-Amino-3,5-cyclohexadiene-1,2-dione, 9CI



$C_6H_5NO_2$ M 123.1
Blue-black soln. in anhyd. EtOAc. Too unstable to isolate. Forms a radical anion identified by esr.

[80314-27-8]

Boyer, J.H. *et al*, *J.A.C.S.*, 1960, **82**, 4748.
Murphy, D. *et al*, *J.C.S. Faraday 2*, 1981, **77**, 1589 (*synth, esr*)

4-Amino-1,2-benzoquinone A-1-00058

4-Amino-3,5-cyclohexadiene-1,2-dione, 9CI

[80926-33-6]

$C_6H_5NO_2$ M 123.1
Prepd. *in situ*, not isol. Forms a radical anion identified by esr.

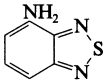
[80314-28-9]

Murphy, D. *et al*, *J.C.S. Faraday 2*, 1981, **77**, 1589 (*synth, esr*)
Solano, F. *et al*, *Biochem. J.*, 1991, **277**, 393.

4-Amino-2,1,3-benzothiadiazole, 8CI A-1-00059

2,1,3-Benzothiadiazol-4-amine, 9CI

[767-64-6]



$C_6H_5N_3S$ M 151.1
Yellow cryst. (H_2O). Mp 67-69°.

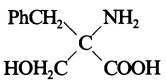
4N-Ac:
$C_8H_7N_3OS$ M 193.2 Cryst. Mp 151-153° (150-151°).

4N-(p-Nitrobenzoyl): Yellow cryst. Mp 207°.
4N-(p-Nitrobenzenesulfonyl): Cryst. Mp 163-164°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1512D.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 580C.
Pesin, V.G. *et al, Zh. Obshch. Khim.*, 1950, **20**, 1914; 1954, **24**, 133; 1958, **28**, 20; *J. Gen. Chem. USSR (Engl. Transl.)*, 1950, **20**, 1981; 1954, **24**, 131; 1958, **28**, 20 (*synth, deriv*)
Efros, L.S. *et al, Zh. Obshch. Khim.*, 1955, **25**, 199; *J. Gen. Chem. USSR (Engl. Transl.)*, 1955, **25**, 183 (*uv*)
Sekikawa, I., *Bull. Chem. Soc. Jpn.*, 1958, **31**, 252 (*synth, deriv synth*)
Belenkaya, I.A. *et al, Khim. Geterotsikl. Soedin.*, 1988, 114; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1988, 96 (*synth*)

2-Amino-2-benzyl-3-hydroxypropanoic acid A-1-00060

α-Benzylserine



$C_{10}H_{13}NO_3$ M 195.2

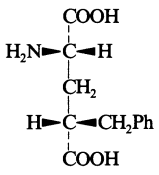
(±)-form

Hydrochloride: Glass.

Zanardi, F. *et al, J.C.S. Perkin 1*, 1995, 2471 (*synth, pmr, cmr, ms*)

2-Amino-4-benzylpentanedioic acid A-1-00061

4-Benzylglutamic acid. 4-(Phenylmethyl) glutamic acid. 2-Amino-4-benzylglutaric acid



$C_{12}H_{15}NO_4$ M 237.2

(2S,4S)-form

Hydrochloride: Solid. Mp 66-68°. $[\alpha]_D$ +11.4 (c, 0.5 in MeOH) (>95% ee).

Ezquerra, J. *et al, J.O.C.*, 1995, **60**, 2925 (*synth, ir, pmr, cmr*)

2-Amino-2-benzyl-3-phenylpropanoic acid A-1-00062

α-Benzylphenylalanine

$(PhCH_2)_2C(NH_2)COOH$

$C_{16}H_{17}NO_2$ M 255.3

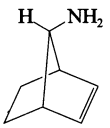
Glassy solid.

N-tert-*Butoxycarbonyl:*
$C_{21}H_{25}NO_4$ M 355.4 Glass.

Zanardi, F. *et al, J.C.S. Perkin 1*, 1995, 2471 (*synth, pmr, cmr*)

1-Aminobicyclo[2.2.1]hept-2-ene A-1-00063

Bicyclo[2.2.1]hept-2-en-7-amine, 9CI. 2-Norbornen-7-amine, 8CI. 7-Amino-2-norbornene



(*1RS,7RS*)-*form*

$C_7H_{11}N$ M 109.1

(1RS,7RS)-form [14173-90-1]
syn-*form*
Oil. Bp_{18} 49-51°. n_D^{28} 1.5062.

Hydrochloride: [35092-57-0].
Needles (Et_2O/MeOH). Mp >250°.

N-*Ac:*
$C_9H_{13}NO$ M 151.2 Needles (hexane). Mp 92.5°.

(1RS,7SR)-form [14173-89-8]
anti-*from*
Waxy solid.

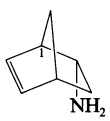
Hydrochloride: Mp >250°.
N-*Ac:* Needles (hexane). Mp 123.5°.

Tanida, H. *et al, J.O.C.*, 1966, **31**, 3941 (*synth, Ac, ir, pmr*)
Marsh, F.D. *et al, J.O.C.*, 1972, **37**, 2969 (*synth*)

5-Aminobicyclo[2.2.1]hept-2-ene A-1-00064

Bicyclo[2.2.1]hept-5-en-2-amine, 9CI. 5-Norbornen-2-amine, 8CI

[52430-93-0]



(*1RS,5RS*)-*form*

$C_7H_{11}N$ M 109.1

(1RS,5RS)-form [77697-44-0]
(±)-endo-*form*
Liq. Bp 152-156°.

N-*Ac:*
$C_9H_{13}NO$ M 151.2 Cryst. (petrol). Mp 93.5-95°.

N,N-*Di-Me:*
$C_9H_{15}N$ M 137.2 Liq. Bp_{17} 65-67°.

(1RS,5SR)-form [18530-45-5]
(±)-exo-*form*
Liq. Bp_{18} 53-54°.

N-*Ac:* [66542-73-2].
Needles ($CHCl_3$/hexane). Mp 112-113°.
N,N-*Di-Me:* Liq. Bp_{20} 66-68°.

Parham, W.E., *J.A.C.S.*, 1951, **73**, 5068; 1952, **74**, 5646 (*synth, Ac*)
Cope, A.C. *et al, J.A.C.S.*, 1959, **81**, 2799 (*N,N-Di-Me*)
Boehme, W.R. *et al, J. Med. Chem.*, 1961, **4**, 183 (*synth*)
Diveley, W.R. *et al, J.A.C.S.*, 1969, **34**, 616 (*synth*)
Bott, S.G. *et al, Synth. Commun.*, 1994, **24**, 3141 (*synth, Ac, ir, pmr, cmr*)

5-Amino-2,2′-bipyridine A-1-00065

[*2,2′-Bipyridine*]-*5-amine, 9CI*

[160539-04-8]

$C_{10}H_9N_3$ M 171.2
Cryst. (toluene). Mp 136°.

Sprecher, M. *et al, Org. Prep. Proced. Int.*, 1994, **26**, 696 (*synth, pmr, cmr, uv, ir, ms*)

3-Amino-2,2-bis(aminomethyl)-1-propanol, 9CI A-1-00066

[120844-28-2]

$(H_2NCH_2)_3CCH_2OH$

$C_5H_{15}N_3O$ M 133.1

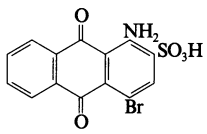
Hydrochloride (1:3): [130147-45-4].
Cryst. (conc. HCl). Mp 298°.

Litherland, A. *et al, J.C.S.*, 1938, 1588 (*synth*)
Neumann, W.L. *et al, J.O.C.*, 1990, **55**, 6368 (*synth*)
Martin, V.V. *et al, Org. Prep. Proced. Int.*, 1995, **27**, 117 (*synth*)

1-Amino-4-bromoanthraquinone-2-sulfonic acid A-1-00067

1-Amino-4-bromo-9,10-dihydro-9,10-dioxo-2-anthracenesulfonic acid, 9CI. Bromoamine acid

[116-81-4]

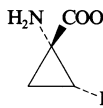


$C_{14}H_8BrNO_5S$ M 382.1
Poorly documented though appears to be a relatively useful compd. Dyestuff intermed. Red needles (H_2O).

[6258-06-6]

Beilsteins Handbuch der Organischen Chemie, 4th edn., 1931, **14**, I 764, II 516.
Zimnicki, J., *Przem. Chem.*, 1984, **63**, 515 (*rev*)

1-Amino-2-bromocyclopropane-carboxylic acid A-1-00068



(*1RS,2RS*)-*form*

$C_4H_6BrNO_2$ M 180.0

(1RS,2RS)-form
(±)-trans-*form*
Cryst. (MeOH/EtOAc) (as hydrochloride). Mp >120° (slow dec.) (hydrochloride).

N-tert-*Butyloxycarbonyl, Me ester:*
$C_{10}H_{16}BrNO_4$ M 294.1 Mp 88-89°.

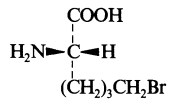
(1RS,2SR)-form
(±)-cis-*form*
Cryst. (MeOH/EtOAc). Mp >120° (slow dec.).

N-tert-*Butyloxycarbonyl, Me ester:* Mp 89-90°.

Wick, L. *et al, Helv. Chim. Acta*, 1995, **78**, 403 (*synth, pmr, cmr, cryst struct*)

2-Amino-6-bromohexanoic acid A-1-00069

6-Bromonorleucine



(*S*)-*form*

$C_6H_{12}BrNO_2$ M 210.0

(*S*)-*form*

L-form

Hydrobromide: [76419-49-3]. Mp 158-159°.

Me ester: [154061-67-3]. $C_7H_{14}BrNO_2$ M 224.0 Cryst. solid (as hydrobromide). Mp 117-118°.

N-*Ac*, *Me ester:* [154061-68-4]. $C_9H_{16}BrNO_3$ M 266.1 Oil.

(±)-*form*

Solid. Mp 151-152°.

Hydrobromide: [10308-06-2]. Solid. Mp 158-159°.

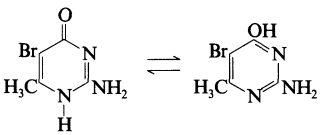
[76419-49-3]

Ermolaev, K.M. *et al*, *CA*, 1966, **65**, 9013a (*synth*)
Effenberger, F. *et al*, *Chem. Ber.*, 1981, **114**, 173 (*synth*)
Mihara, H. *et al*, *CA*, 1984, **100**, 34793j (*synth*)
Bambal, R. *et al*, *J.O.C.*, 1994, **59**, 729 (*deriv, synth, pmr, cmr*)

2-Amino-5-bromo-4-hydroxy-6-methylpyrimidine A-1-00070

2-Amino-5-bromo-6-methyl-4(1H)-pyrimidinone, 9CI. 2-Amino-5-bromo-6-methyl-4-pyrimidinol, 8CI. 5-Bromo-6-methylisocytosine. U 25166

[6307-35-3]



$C_5H_6BrN_3O$ M 204.0

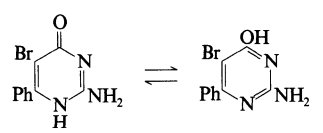
Inducer of interferon. Antiviral agent. Cryst. (H_2O). Mp 250° dec.

Hull, R. *et al*, *J.C.S.*, 1947, 41 (*synth*)
Nishiwaki, T., *Chem. Pharm. Bull.*, 1961, 38 (*synth*)
Ger. Pat., 2 522 047, (1975) (*Upjohn*); *CA*, **84**, 111652t (*synth, pharmacol*)
Nichol, F.R. *et al*, *Antimicrob. Agents Chemother.*, 1976, **9**, 433 (*pharmacol*)
Stringfellow, D.A., *Antimicrob. Agents Chemother.*, 1977, **11**, 984 (*pharmacol*)
Hirota, K. *et al*, *J.O.C.*, 1978, **43**, 1193 (*synth*)
Stringfellow, D.A., *Science (Washington, D.C.)*, 1978, **201**, 376 (*pharmacol*)

2-Amino-5-bromo-4-hydroxy-6-phenylpyrimidine A-1-00071

2-Amino-5-bromo-6-phenyl-4(1H)-pyrimidinone, 9CI. 2-Amino-5-bromo-6-phenyl-4-pyrimidinol. ***Bropirimine, BAN, INN, USAN.*** *U 54461. ABPP*

[56741-95-8]



$C_{10}H_8BrN_3O$ M 266.0

Antineoplastic and antiviral agent, interferon-alpha inducer. Shows antifibrotic activity in animal model of lung fibrosis. Phase II clinical trial (1993). Cryst. (EtOH aq.). Mp 268-270° (246-248°).

▶ LD_{50} (rat, orl) >3200 mg/kg. Exp. reprod. and teratogenic effects. Mutagenic props. UW7351300.

Brown, T.B. *et al*, *J.C.S. Perkin 1*, 1975, 1023 (*synth*)
Wynalda, M.A. *et al*, *Anal. Chem.*, 1980, **52**, 1931 (*hplc*)
Stringfellow, D.A., *Prog. Cancer Res. Ther.*, 1981, **16**, 215 (*pharmacol*)
Wierenga, W., *Drugs of the Future*, 1984, **9**, 567 (*rev*)
Skulnick, H.I. *et al*, *J. Med. Chem.*, 1985, **28**, 1864 (*synth, pharmacol*)
Aaron, C.S. *et al*, *Mutat. Res.*, 1991, **252**, 221, 229, 239 (*tox*)
Zia, S. *et al*, *Pharmacol. Toxicol.*, 1992, **71**, 11.
Wierenga, W., *Ann. N.Y. Acad. Sci.*, 1993, **685**, 296, 301 (*rev*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, AIY850.

2-Aminobutanal A-1-00072

$H_3CCH_2CH(NH_2)CHO$

C_4H_9NO M 87.1

(±)-*form*

N,N-*Di-Me:* [20068-48-8]. $C_6H_{13}NO$ M 115.1 Bp_{18} 44-45°, Bp_{16} 36°. n_D^{24} 1.424.

N,N-*Di-Et:* [20493-63-4]. $C_8H_{17}NO$ M 143.2 Bp_{12} 53°.

Kogl, F. *et al*, *Annalen*, 1942, **552**, 1 (*Di-Me*)
Kirrman, A. *et al*, *Bull. Soc. Chim. Fr.*, 1968, 1091 (*Di-Et*)
Duhamel, L. *et al*, *Bull. Soc. Chim. Fr.*, 1968, 2942 (*Di-Me synth, ir, pmr*)

3-Aminobutanal, 9CI A-1-00073

$H_3CCH(NH_2)CH_2CHO$

C_4H_9NO M 87.1

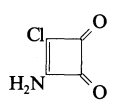
(±)-*form*

Bp_{12} 48°.

Birkofer, L. *et al*, *Chem. Ber.*, 1958, **91**, 2383 (*synth*)

3-Amino-4-chloro-3-cyclobutene-1,2-dione, 9CI A-1-00074

[97962-64-6]



$C_4H_2ClNO_2$ M 131.5

Cryst. (AcOH). Mp 180°.

N,N-*Di-Me:* [37669-68-4]. *3-Chloro-4-(dimethylamino)-3-cyclobutene-1,2-dione, 9CI*
$C_6H_6ClNO_2$ M 159.5 Light yellow cryst. Mp 74-76°.

N,N-*Di-Et:* [147932-81-8]. *3-Chloro-4-(diethylamino)-3-cyclobutene-1,2-dione*
$C_8H_{10}ClNO_2$ M 187.6 Deep yellow cryst. Mp 49.2-53.3°.

N-*Ph:* [97962-70-4].
$C_{10}H_6ClNO_2$ M 207.6 Yellow cryst. Mp 186-189°.

N-*Ph*, N-*Me:*
$C_{11}H_8ClNO_2$ M 221.6 Yellow cryst. (EtOH). Mp 138-139°.

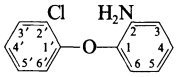
N-*Benzyl*, N-*Ph:* [97962-52-2].
$C_{17}H_{12}ClNO_2$ M 297.7 Light yellow cryst. (EtOH). Mp 85-87°.

Schmidt, A.H. *et al*, *Annalen*, 1985, 1021 (*synth, deriv*)
Schmidt, A.H. *et al*, *Synthesis*, 1987, 134.
Ohno, M. *et al*, *J.C.S. Perkin 1*, 1993, 263 (*di-Et deriv, synth, ir, pmr, cmr, ms*)

2-Amino-2′-chlorodiphenyl ether A-1-00075

2-(2-Chlorophenoxy)benzenamine, 9CI. 2-(2-Chlorophenoxy)aniline

[56966-47-3]



$C_{12}H_{10}ClNO$ M 219.6

Prisms (petrol). Mp 45°. Bp_{15} 203°.

Hydrochloride: Plates. Mp 171-173°.

Roberts, E., *J.C.S.*, 1925, **127**, 2004.
McCombie, H. *et al*, *J.C.S.*, 1931, 529.

2-Amino-3′-chlorodiphenyl ether A-1-00076

2-(3-Chlorophenoxy)benzenamine. 2-(3-Chlorophenoxy)aniline

[76838-73-8]

$C_{12}H_{10}ClNO$ M 219.6

Bp_{13} 195°.

Hydrochloride: Prisms. Mp 149-151°.

N-*Benzoyl:*
$C_{19}H_{14}ClNO_2$ M 323.7 Needles (EtOH aq.). Mp 106°.

Roberts, E., *J.C.S.*, 1925, **127**, 2004.

2-Amino-4′-chlorodiphenyl ether A-1-00077

2-(4-Chlorophenoxy)benzenamine. 2-(4-Chlorophenoxy)aniline

[2770-11-8]

$C_{12}H_{10}ClNO$ M 219.6

Bp_{15} 202°, $Bp_{0.1}$ 118°.

Hydrochloride: [114709-63-6]. Prisms or needles. Mp 190-191° (181°).

N-*Benzoyl:*
$C_{19}H_{14}ClNO_2$ M 323.7 Fine needles (EtOH aq.). Mp 108-109°.

Roberts, E. *et al*, *J.C.S.*, 1925, 2004.
McCombie, H. *et al*, *J.C.S.*, 1931, 529.
Wardrop, A.W.H. *et al*, *J.C.S. Perkin 1*, 1976, 1279.

4-Amino-4′-chlorodiphenyl ether A-1-00078

4-(4-Chlorophenoxy)benzenamine. 4-(4-Chlorophenoxy)aniline

[101-79-1]

$C_{12}H_{10}ClNO$ M 219.6

Prisms (MeOH). Mp 98-100°.

N-*Ac:*
$C_{14}H_{12}ClNO_2$ M 261.7 Plates (MeOH). Mp 146°.

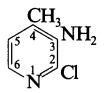
[40859-51-6]

Scarborough, H.A., *J.C.S.*, 1929, 2361.

3-Amino-2-chloro-4-methylpyridine A-1-00079

2-Chloro-4-methyl-3-pyridinamine

[133627-45-9]



$C_6H_7ClN_2$ M 142.5
Cryst. (EtOAc). Mp 65-66°.

Hargrave, K.D. *et al*, *J. Med. Chem.*, 1991, **34**, 2231 (*synth, pmr*)
Grozinger, K.G. *et al*, *J. Het. Chem.*, 1995, **32**, 259 (*synth*)

3-Amino-2-chloro-6-methylpyridine A-1-00080

2-Chloro-6-methyl-3-pyridinamine

[39745-40-9]

$C_6H_7ClN_2$ M 142.5
Cryst. (diisopropyl ether/petrol). Mp 76-78°.

Tomczuk, B.E. *et al*, *J. Med. Chem.*, 1991, **34**, 2993 (*synth*)

4-Amino-3-chloro-2-methylpyridine A-1-00081

3-Chloro-2-methyl-4-pyridinamine

[97944-40-6]

$C_6H_7ClN_2$ M 142.5
Cryst. ($CHCl_3$/petrol). Mp 108-110°.

Ife, R.J. *et al*, *J. Med. Chem.*, 1989, **32**, 1970 (*synth, pmr*)

5-Amino-2-chloro-4-methylpyridine A-1-00082

6-Chloro-4-methyl-3-pyridinamine

[66909-38-4]

$C_6H_7ClN_2$ M 142.5

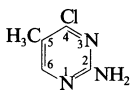
Ac:
$C_8H_9ClN_2O$ M 184.6 Cryst. Mp 155-156°.

Chapman, D. *et al*, *J.C.S. Perkin 1*, 1980, 2398 (*synth, pmr*)

2-Amino-4-chloro-5-methylpyrimidine A-1-00083

4-Chloro-5-methyl-2-pyrimidinamine, 9CI

[20090-58-8]



$C_5H_6ClN_3$ M 143.5
Needles (EtOH). Mp 184-185°.

Hull, R. *et al*, *J.C.S.*, 1947, 41 (*synth*)

2-Amino-4-chloro-6-methylpyrimidine, 8CI A-1-00084

4-Chloro-6-methyl-2-pyrimidinamine, 9CI

[5600-21-5]

$C_5H_6ClN_3$ M 143.5
Nitrification inhibitor. Cryst. (EtOH). Mp 183-186°.

Gabriel, S. *et al*, *Ber.*, 1899, **32**, 2921 (*synth*)
Johnson, T.B. *et al*, *J.A.C.S.*, 1938, **60**, 1622 (*synth*)
Clews, C.J.B. *et al*, *Nature (London)*, 1947, **159**, 264 (*cryst struct*)
Marshall, J.R. *et al*, *J.C.S.*, 1951, 1004 (*synth*)
Slangen, J.H.G., *Fert. Res.*, 1984, **5**, 1 (*rev, use*)

4-Amino-5-chloro-2-methylpyrimidine A-1-00085

5-Chloro-2-methyl-4-pyrimidinamine

$C_5H_6ClN_3$ M 143.5
Cryst. Mp 145-146°.

Budesinsky, Z., *Coll. Czech. Chem. Comm.*, 1949, **14**, 223 (*synth*)

4-Amino-5-chloro-6-methylpyrimidine A-1-00086

5-Chloro-6-methyl-4-pyrimidinamine

$C_5H_6ClN_3$ M 143.5
Prisms (H_2O). Mp 197-198°.

Gabriel, S. *et al*, *Ber.*, 1901, **34**, 1238 (*synth*)
Nishiwaki, T., *Tetrahedron*, 1966, **22**, 2401 (*synth*)

4-Amino-6-chloro-2-methylpyrimidine A-1-00087

6-Chloro-2-methyl-4-pyrimidinamine, 9CI

[1749-68-4]

$C_5H_6ClN_3$ M 143.5
Needles (MeOH). Mp 190-191°.

Foldi, Z. *et al*, *Ber., B*, 1942, **75**, 755 (*synth*)
Baddiley, J. *et al*, *J.C.S.*, 1943, 383 (*synth*)

4-Amino-6-chloro-5-methylpyrimidine A-1-00088

6-Chloro-5-methyl-4-pyrimidinamine

[14394-56-0]

$C_5H_6ClN_3$ M 143.5
Cryst. (H_2O). Mp 237-238°.

Hull, R. *et al*, *J.C.S.*, 1947, 41.

5-Amino-2-chloro-4-methylpyrimidine A-1-00089

2-Chloro-4-methyl-5-pyrimidinamine

[20090-69-1]

$C_5H_6ClN_3$ M 143.5
Needles (H_2O). Mp 93.5°.

Gabriel, S. *et al*, *Ber.*, 1901, **34**, 1238 (*synth*)
Overberger, C.G. *et al*, *J.A.C.S.*, 1954, **76**, 1953 (*synth*)

5-Amino-4-chloro-6-methylpyrimidine A-1-00090

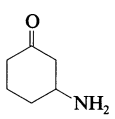
4-Chloro-6-methyl-5-pyrimidinamine

$C_5H_6ClN_3$ M 143.5
Cryst. Mp 98-99°.

Taylor, E.C. *et al*, *J.O.C.*, 1961, **26**, 4961 (*synth*)

3-Aminocyclohexanone A-1-00091

[149520-74-1]



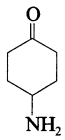
$C_6H_{11}NO$ M 113.1

N,N-*Di-Me:* [15676-74-1]. *3-Dimethylaminocyclohexanone*
$C_8H_{15}NO$ M 141.2 Mp 102-103°.

Mousseron, M. *et al*, *Bull. Soc. Chim. Fr.*, 1954, 1246 (*deriv*)
U.S. Pat., 5 206 367, (1993); *CA*, **119**, 139228z (*synth*)

4-Aminocyclohexanone A-1-00092

[87976-86-1]



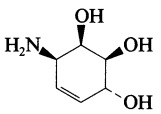
$C_6H_{11}NO$ M 113.1
Parent compd. poorly documented, not characterised.

N,N-*Di-Me:* [40594-34-1].
$C_8H_{15}NO$ M 141.2 Bp_{12} 95°. n_D^{25} 1.4706.

Nelson, N.A. *et al*, *J.O.C.*, 1957, **22**, 1146 (*deriv*)
Sola, R. *et al*, *Nouv. J. Chim.*, 1984, **8**, 459; *CA*, **102**, 45224s.

6-Amino-4-cyclohexene-1,2,3-triol A-1-00093

[89615-00-9]



(1*R*,2*S*,3*R*,6*R*)-*form*

$C_6H_{11}NO_3$ M 145.1

(1R,2S,3R,6R)-form [142796-97-2]
V. hygroscopic solid. Mp 148-150° (90-92°). $[\alpha]_D^{25}$ −221 (c, 0.79 in MeOH).

(1RS,2RS,3RS,6SR)-form
Conduramine F_4
No phys. props. reported.

(1RS,2RS,3SR,6RS)-form [155239-03-5]
Conduramine F_1

N,O,O,O-*Tetra-Ac:*
$C_{14}H_{19}NO_7$ M 313.3 Mp 142° (139-141°).

(1RS,2SR,3RS,6RS)-form [155239-06-8]
Conduramine C_1
Cryst.

(1RS,2SR,3RS,6SR)-form [155239-00-2]
Conduramine A_1

N,O,O,O-*Tetra-Ac:* Mp 156-159° (121°).

(1RS,2SR,3SR,6SR)-form
Conduramine C_4
No phys. props. reported.

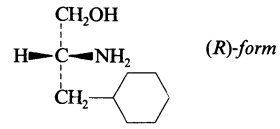
[78774-27-3, 79435-30-6, 138513-21-0, 139626-79-2, 139626-80-5, 141269-14-9]

Allemann, S. *et al*, *Helv. Chim. Acta*, 1994, **77**, 1 (*synth, bibl*)
Leung-Toung, R. *et al*, *Tet. Lett.*, 1994, **35**, 1639 (*synth, bibl*)

2-Amino-3-cyclohexylpropanol A-1-00094

β-Aminocyclohexanepropanol, 9CI. Cyclohexylalaninol

[103808-94-2]



(*R*)-*form*

$C_9H_{19}NO$ M 157.2

(*R*)-*form*

Mp 152-154° (hydrochloride). $[\alpha]_D^{20}$ −2.24 (c, 2.99 in H_2O).

(*S*)-*form* [117160-99-3]

L-form

Mp 151-154° (hydrochloride). $[\alpha]_D^{21}$ +2.05 (c, 4.87 in H_2O). CAS no. refers to hydrochloride.

N-tert-*Butyloxycarbonyl:* Thick oil.

[131288-67-0]

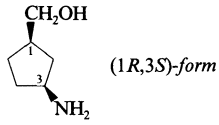
Grunewald, G.L. *et al, J. Med. Chem.*, 1982, **25**, 1248 (*synth*)

Krysan, D.J. *et al, Org. Prep. Proced. Int.*, 1993, **25**, 437.

3-Aminocyclopentanemethanol, 9CI A-1-00095

1-Amino-3-hydroxymethylcyclopentane

[123288-54-0]



(1*R*,3*S*)-*form*

$C_6H_{13}NO$ M 115.1

Precursor to synth. of carbocyclic nucleosides.

(*1R,3S*)-*form* [117957-62-7]

Described as (1*S*,3*R*) by Bergmeier.

Hydrochloride: [147780-38-9].

Glass. $[\alpha]_D^{20}$ −7.4 (c, 2.7 in 1*M* HCl).

N-*Phenylsulfonyl:* [151112-65-1].

$[\alpha]_D^{25}$ −4.5 (c, 1.5 in $CHCl_3$).

(*1S,3S*)-*form*

Hydrochloride: [147780-45-8].

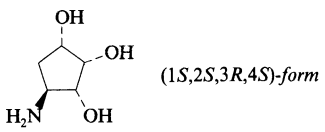
Oil. $[\alpha]_D^{20}$ −2.7 (c, 2.2 in 1*M* HCl).

[78795-20-7, 102099-18-3, 151214-31-2]

Hronowski, L.J.J. *et al, Can. J. Chem.*, 1988, **66**, 61 (*synth, pmr*)

Bergmeier, S.C. *et al, J.O.C.*, 1993, **58**, 2369, 5019 (*synth, pmr, cmr*)

4-Amino-1,2,3-cyclopentanetriol A-1-00096



(1*S*,2*S*,3*R*,4*S*)-*form*

$C_5H_{11}NO_3$ M 133.1

(*1S,2S,3R,4S*)-*form*

2,3-O-Isopropylidene:

$C_8H_{15}NO_3$ M 173.2 Synthon for carbocyclic nucleosides e.g. Aristeromycin, A-0-04394. Mp 85.8°. $[\alpha]_D$ −51.5 (c, 0.33 in $CHCl_3$).

(*1RS,2RS,3SR,4RS*)-*form*

2,3-O-Isopropylidene: Mp 128°.

(*1RS,2SR,3RS,4SR*)-*form*

2,3-O-Isopropylidene: Cryst. (Et_2O). Mp 128°.

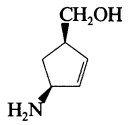
Jung, M. *et al, Helv. Chim. Acta*, 1983, **66**, 1915 (*synth, ir, pmr*)

Gallos, J.K. *et al, J.C.S. Perkin 1*, 1994, 613 (*synth*)

4-Amino-2-cyclopentene-1-methanol A-1-00097

2-Amino-4-hydroxymethylcyclopentene. 4-Hydroxymethyl-2-cyclopenten-1-amine

[121481-90-1]



$C_6H_{11}NO$ M 113.1

(*1RS,4SR*)-*form* [122624-72-0]

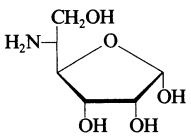
(±)-cis-*form*

Syrup. Not purified.

[131320-53-1, 136522-30-0, 136522-35-5]

Norman, M.H. *et al, Synth. Commun.*, 1992, **22**, 3197 (*synth*)

5-Amino-5-deoxyallose A-1-00098



α-D-Furanose-*form*

$C_6H_{13}NO_5$ M 179.1

α-D-*Furanose-form*

1,2-O-Isopropylidene, 3,5N-dibenzoyl: [31718-81-7].

$C_{23}H_{25}NO_7$ M 427.4 Mp 206-208°. $[\alpha]_D^{22}$ +100 (c, 1.2 in $CHCl_3$).

1,2-O-Isopropylidene, 3,5N-dibenzoyl, 6-trityl: [31718-80-6].

$C_{42}H_{39}NO_7$ M 669.7 Syrup. $[\alpha]_D^{22}$ +67 (c, 1.1 in $CHCl_3$).

β-D-*Furanose-form*

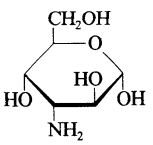
Allyl glycoside, 2,3-O-isopropylidene: [123168-75-2].

$C_{12}H_{21}NO_5$ M 259.3 Solid. Mp 83.5-84.5°. $[\alpha]_D^{20}$ −46.5 (c, 0.72 in CH_2Cl_2).

Naka, T. *et al, Tet. Lett.*, 1971, 95 (α-D-fur deriv, pmr)

Auberson, Y. *et al, Angew. Chem., Int. Ed.*, 1989, **28**, 1498 (*allyl glycoside, ir*)

3-Amino-3-deoxyaltrose A-1-00099



α-D-Pyranose-*form*

$C_6H_{13}NO_5$ M 179.1

α-D-*Pyranose-form*

Me glycoside: [55274-73-2].

$C_7H_{15}NO_5$ M 193.1 Mp 208° (188°) dec. (hydrochloride). $[\alpha]_D^{25}$ +91 (c, 1.1 in H_2O). CAS no. refers to hydrochloride.

Me glycoside, 2,3N,4,6-tetra-Ac: [72523-30-9].

$C_{15}H_{23}NO_9$ M 361.3 Cryst. (EtOAc/$CHCl_3$). Mp 177° (171-172°). $[\alpha]_D$ +42.2 ($CHCl_3$).

β-D-*Pyranose-form*

Benzyl glycoside:

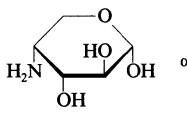
$C_{13}H_{19}NO_5$ M 269.2 Cryst. (EtOH) (as hydrochloride). Mp 200-250° dec. (hydrochloride). $[\alpha]_D^{25}$ −72 (c, 0.5 in D_2O).

Baker, B.R. *et al, J.O.C.*, 1954, **19**, 646 (*α-Me pyr tetra-Ac*)

Baer, H.H. *et al, Carbohydr. Res.*, 1979, **76**, 141 (*α-Me pyr*)

Jacobsen, S., *Acta Chem. Scand., Ser. B*, 1988, **42**, 605 (*α-Me pyr deriv*)

4-Amino-4-deoxyarabinose A-1-00100



α-D-Pyranose-*form*

$C_5H_{11}NO_4$ M 149.1

D-form [86288-09-7]

Constit. of lipopolysaccharide of some gram negative bacteria e.g. *Salmonella minnesota, S. typhimurium, Proteus mirabilis, Rhodocyclus purpureus.*

N-*Ac:*

$C_7H_{13}NO_5$ M 191.1 Cryst. (MeOH/Et_2O). Mp 157.5-158.5°. $[\alpha]_D^{23}$ −65 → −73 (c, 2.53 in H_2O).

α-D-*Pyranose-form*

Me glycoside: Methyl 4-amino-4-deoxy-α-D-arabinopyranoside

$C_6H_{13}NO_4$ M 163.1 Cryst. (EtOH) (as hydrochloride). Mp 180-183° (hydrochloride). $[\alpha]_D^{23}$ +3 (c, 1.75 in H_2O).

Me glycoside, N-*Ac:*

$C_8H_{15}NO_5$ M 205.2 Cryst. (EtOH). Mp 129-130°. $[\alpha]_D^{23}$ +1.6 (c, 1.83 in H_2O).

α-D-*Furanose-form*

1,2,3,4N, 5-Penta-Ac:

$C_{15}H_{21}NO_9$ M 359.3 Syrup. $[\alpha]_D^{23}$ −31 (c, 0.45 in $CHCl_3$).

Me glycoside, N-*Ac:* Cryst. (MeOH/Et_2O/heptane). Mp 145.5-146.5°. $[\alpha]_D^{23}$ −44 (c, 1 in H_2O).

β-D-*Furanose-form*

1,2,3,4N, 5-Penta-Ac: Syrup. $[\alpha]_D^{23}$ −70 (c, 1.35 in $CHCl_3$).

Me glycoside, N-*Ac:* Syrup. $[\alpha]_D^{23}$ −68 (c, 0.5 in H_2O).

L-Pyranose-form

Hydrochloride: Yellow glass. $[\alpha]_D^{20}$ +49.6 (c, 0.8 in D_2O).

α-L-*Pyranose-form*

Me glycoside: [19140-34-2]. *Methyl 4-amino-4-deoxy-α-L-arabinopyranoside*

$C_6H_{13}NO_4$ M 163.1 Cryst. (as hydrochloride). Mp 184.5-185° dec. (hydrochloride). $[\alpha]_D$ −3 (c, 0.98 in H_2O). CAS no. refers to hydrochloride.

Me glycoside, N-*Ac:* [19140-35-3]. Cryst. Mp 129-130°. $[\alpha]_D$ −1.8 (c, 3.43 in H_2O).

Me glycoside, 2,3,4N-tri-Ac: [19210-07-2].

$C_{12}H_{19}NO_7$ M 289.2 Glass. $[\alpha]_D$ −34 (c, 1.35 in $CHCl_3$).

β-L-*Pyranose-form*

1-Dihydrogen phosphate: [83364-05-0].

$C_5H_{12}NO_7P$ M 229.1 Constit. of lipopolysaccharide of *Salmonella minnesota*. Syrup.

*Me glycoside, 2,3,4*N*-tri-Ac:* [76800-61-8]. Prisms + $0.5H_2O$ (EtOAc/hexane). Mp 72-75°.

Me glycoside, 2,3-dimesyl, N*-Ac:* [89195-93-7].
$C_{10}H_{19}NO_9S_2$ M 361.3 Prisms (pentane). Mp 162-163° (158-159°).

[29973-49-7, 118117-12-7, 118149-40-9]

Dick, A.J. *et al, Can. J. Chem.*, 1968, **46**, 425 (D-deriv, α-D-pyr derivs, α-D-fur derivs, β-D-fur derivs, α-L-pyr derivs)

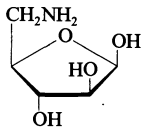
Batley, M. *et al, Biochemistry*, 1982, **21**, 6580 (*phosphate, pmr, occur*)

Nateway, J.J. *et al, Carbohydr. Res.*, 1988, **179**, 199 (L-pyr)

Bhat, R. *et al, J. Bacteriol.*, 1990, **172**, 6631 (*occur*)

Dimitriev, B.A. *et al, FEMS Microbiol. Lett.*, 1991, **77**, 39 (*occur*)

5-Amino-5-deoxyarabinose A-1-00101



β-D-Furanose-*form*

$C_5H_{11}NO_4$ M 149.1

β-D-Furanose-form

1,2-O-Isopropylidene, 3-mesyl, N*-Ac:* [7687-67-4].
$C_{11}H_{19}NO_7S$ M 309.3 Cryst. (Me_2CO/Et_2O/pentane). Mp 127-128°. $[\alpha]_D^{25}$ +6.5 (c, 1.16 in MeOH).

1,2-O-Isopropylidene, 3-mesyl, N*-benzoyl:* [7687-68-5].
$C_{16}H_{21}NO_7S$ M 371.4 Mp 117-118°. $[\alpha]_D^{25}$ +9 (c, 0.55 in MeOH).

L-form

5N-*Ac, benzylphenylhydrazone:* Cryst. (Me_2CO/Et_2O/pentane). Mp 155-156°. $[\alpha]_D^{23}$ −12.2 (c, 2.05 in MeOH).

1-Diethyldithioacetal, N*-Ac:*
$C_{11}H_{23}NO_4S_2$ M 297.4 Cryst. (EtOH/Et_2O/2,2,4-trimethylpentane). Mp 133-134°. $[\alpha]_D^{23}$ +90 (c, 1.0 in $CHCl_3$).

L-Pyranose-form

N-*Ac:* [13428-12-1].
$C_7H_{13}NO_5$ M 191.1 Mp 145-146°. $[\alpha]_D^{24}$ +18.5 (c, 2.02 in H_2O), $[\alpha]_D^{24}$ +8.6 (0.1*M* HCl).

L-Furanose-form

*1,2,3,5*N*-Tetra-Ac:*
$C_{13}H_{19}NO_8$ M 317.2 Syrup. $[\alpha]_D$ +5 (c, 2.62 in $CHCl_3$).

β-L-Furanose-form

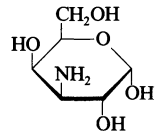
1,2-O-Isopropylidene, N*-Ac:*
$C_{10}H_{17}NO_5$ M 231.2 Cryst. Mp 143-144°. $[\alpha]_D$ −45 (c, 2.0 in MeOH).

Jones, J.K.N. *et al, J.C.S.*, 1962, 4699 (L-form, β-L-fur)

Hanessian, S. *et al, J.O.C.*, 1963, **28**, 2604 (L-form, L-pyr)

Hanessian, S. *et al, J.O.C.*, 1967, **32**, 163 (β-D-fur)

3-Amino-3-deoxygalactose A-1-00102



α-D-Pyranose-*form*

$C_6H_{13}NO_5$ M 179.1

α-D-Pyranose-form

Me glycoside: [122204-77-7].
$C_7H_{15}NO_5$ M 193.1 Cryst. Mp 96-99°.

Me glycoside, hydrochloride: [37073-85-1]. Mp 219-221° (197°) dec. $[\alpha]_D^{20}$ +159 (c, 0.3 in H_2O).

*Me glycoside, 2,3*N*,4,6-tetra-Ac:*
$C_{15}H_{23}NO_9$ M 361.3 Syrup. $[\alpha]_D$ +104 (c, 0.6 in $CHCl_3$).

β-D-Pyranose-form

N-*Ac:* [135684-04-7].
$C_8H_{15}NO_6$ M 221.2 Cryst. (MeOH). Mp 173-174°. $[\alpha]_D$ +99 → +119 (c, 2.5 in H_2O).

1,6-Anhydro:
$C_6H_{11}NO_4$ M 161.1 Cryst. (MeOH/Me_2CO) (as hydrochloride). Mp 180-185° dec. (hydrochloride). $[\alpha]_D^{20}$ −9.0 (c, 1.0 in H_2O).

Kuhn, R. *et al, Annalen*, 1960, **636**, 164 (*β-N-Ac*)

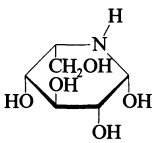
Heyns, K. *et al, Chem. Ber.*, 1965, **98**, 327 (*anhydro*)

Baer, H.H. *et al, Can. J. Chem.*, 1972, **50**, 1216 (*α-Me pyr*)

Jacobsen, S., *Acta Chem. Scand., Ser. B*, 1988, **42**, 605 (*deriv, pmr, cmr*)

Defaye, J. *et al, Carbohydr. Res.*, 1991, **212**, 129 (*α-N-Ac, β-N-Ac, pmr, cmr*)

5-Amino-5-deoxyidose A-1-00103



β-L-Pyranose-*form*

$C_6H_{13}NO_5$ M 179.1

β-L-Pyranose-form

1,6-Anhydro: [15065-80-2].
$C_6H_{11}NO_4$ M 161.1 Cryst. (MeOH). Mp 140° dec. $[\alpha]_D^{23}$ +114.5 (c, 1.0 in H_2O).

1,6-Anhydro, N*-Ac:* [14679-59-5].
$C_8H_{13}NO_5$ M 203.1 Cryst. (MeOH). Mp 190-191°. $[\alpha]_D^{20}$ +79.3 (c, 2.0 in H_2O).

*1,6-Anhydro, 2,3,4,5*N*-tetra-Ac:* [15072-72-7].
$C_{14}H_{19}NO_8$ M 329.3 Syrup. $[\alpha]_D^{20}$ +48.9 (c, 2.0 in MeOH).

β-L-Furanose-form

1,2-O-Isopropylidene: [14685-99-5].
$C_9H_{17}NO_5$ M 219.2 Leaflets (EtOH/Et_2O). Mp 184-185° (178°). $[\alpha]_D^{20}$ −3.7 (c, 1.1 in MeOH).

*1,2-O-Isopropylidene, 3,5*N*,6-tri-Ac:* [25474-01-5].
$C_{15}H_{23}NO_8$ M 345.3 Cryst. (Et_2O). Mp 92-94°. $[\alpha]_D^{23}$ −14.4 (c, 2.3 in $CHCl_3$).

1,2-O-Isopropylidene, 3-benzyl, N*-Ac:* [22412-62-0].
$C_{18}H_{25}NO_6$ M 351.3 Needles (2-propanol/hexane). Mp 143-144°. $[\alpha]_D^{21}$ −7.4 (c, 5.3 in $CHCl_3$).

1,2-O-Isopropylidene, N*-benzyloxycarbonyl:* [129279-37-4].
$C_{17}H_{23}NO_7$ M 353.3 Cryst. (EtOAc). Mp 140-141°. $[\alpha]_D$ −24.5 (c, 0.5 in $CHCl_3$).

Gramera, R.E. *et al, J.O.C.*, 1963, **28**, 1401 (*isopropylidene*)

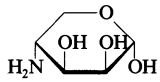
Paulsen, H. *et al, Chem. Ber.*, 1966, **99**, 3450 (β-L-pyr deriv)

Saeki, H. *et al, Chem. Pharm. Bull.*, 1968, **16**, 962, 2471 (*isopropyldiene, ir*)

Tsuda, Y. *et al, Chem. Pharm. Bull.*, 1989, **37**, 2673 (*tri-Ac, ir, pmr, cmr*)

Kayakiri, H. *et al, Chem. Pharm. Bull.*, 1991, **39**, 1397 (*N-benzyloxycarbonyl, pmr, cmr, ms*)

4-Amino-4-deoxylyxose A-1-00104



α-D-Pyranose-*form*

$C_5H_{11}NO_4$ M 149.1

α-D-Pyranose-form

Benzyl glycoside, 2,3-anhydro: [78907-34-3].
$C_{12}H_{15}NO_3$ M 221.2 Cryst. $[\alpha]_D^{20}$ +91 ($CHCl_3$).

α-L-Pyranose-form

Me glycoside, 2-mesyl: [101305-43-5].
$C_7H_{15}NO_6S$ M 241.2 Cryst. (EtOAc). Mp 134°. $[\alpha]_{365}^{25}$ −99 (c, 0.53 in $CHCl_3$).

Me glycoside, N,N-*di-Me, 2,3-dimesyl:* [87908-09-6].
$C_{10}H_{21}NO_8S_2$ M 347.4 Cryst. Mp 118°.

β-L-Pyranose-form

Benzyl glycoside, 2,3-anhydro: [78907-33-2]. Cryst. Mp 37-38°. $[\alpha]_D^{20}$ +105 ($CHCl_3$).

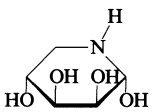
L-Furanose-form [28441-49-8]
Amorph. powder (MeOH). $[\alpha]_D$ +4 (c, 0.92 in H_2O).

Paulsen, H. *et al, Chem. Ber.*, 1970, **103**, 1621 (L-fur)

Picq, D. *et al, Tetrahedron*, 1983, **39**, 1797; 1985, **41**, 2681 (*Me gly deriv, pmr*)

Malik, A. *et al, Chem. Comm.*, 1984, 1530 (*benzyl gly deriv*)

5-Amino-5-deoxylyxose A-1-00105



α-D-Pyranose-*form*

$C_5H_{11}NO_4$ M 149.1

D-form

N-*Ac, benzylphenylhydrazone:* [13391-66-7]. Cryst. (Me_2CO/Et_2O). Mp 155-156°. $[\alpha]_D^{23}$ +23.4 (c, 0.17 in MeOH).

α-D-Pyranose-form

N-*Ac:* [7687-55-0].
$C_7H_{13}NO_5$ M 191.1 Mp 166-167° (156-158°). $[\alpha]_D^{25}$ −71 (c, 1.0 in H_2O), $[\alpha]_D$ −55 (c, 1.0 in H_2O).

*1,2,3,4,5*N*-Penta-Ac:* [7700-00-7].
$C_{15}H_{21}NO_9$ M 359.3 Mp 131-132° (121-122°). $[\alpha]_D$ −20 (c, 0.6 in $CHCl_3$).

α-D-Furanose-form

2,3-O-Isopropylidene, N*-Ac:* [20750-25-8].
$C_{10}H_{17}NO_5$ M 231.2 Cryst. (EtOAc). Mp 125-125.5°. $[\alpha]_D$ +23 (c, 1.0 in MeOH).

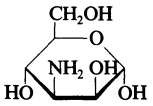
Benzyl glycoside, N*-Ac:* [20750-26-9].

$C_{14}H_{19}NO_5$ M 281.3 Syrup. $[\alpha]_D$ +84 (c, 0.9 in MeOH).

Benzyl glycoside, 2,3-O-isopropylidene, N-Ac: [20750-24-7].
$C_{17}H_{23}NO_5$ M 321.3 Cryst. ($CHCl_3$/petrol). Mp 86-87°. $[\alpha]_D$ +84 (c, 1.0 in $CHCl_3$).

Hanessian, S., *J.O.C.*, 1967, **32**, 163 (*synth, derivs*)
Brimacombe, J.S. *et al, J.C.S.(C)*, 1968, 181 (α-D-fur deriv)
Poh, B. *et al, Aust. J. Chem.*, 1984, **37**, 971 (α-D-pyr deriv, pmr, ir)

3-Amino-3-deoxymannose A-1-00106



α-D-Pyranose-*form*

$C_6H_{13}NO_5$ M 179.1

α-D-Pyranose-form

Hydrochloride: [32795-22-5].
Cryst. Mp 165-167° dec. $[\alpha]_D^{20}$ +17 → 6 (c, 1.0 in H_2O).

1,2,4,6-Tetra-Ac: [33034-49-0].
$C_{14}H_{21}NO_9$ M 347.3 Syrup (as hydrochloride). CAS no. refers to hydrochloride.

1,3N,4,6-Tetra-Ac: [32795-23-6].
$C_{14}H_{21}NO_9$ M 347.3 Cryst. Mp 142-143°. $[\alpha]_D^{20}$ +98 (c, 0.9 in H_2O).

1,2,3N,4,6-Penta-Ac: [33034-50-3].
$C_{16}H_{23}NO_{10}$ M 389.3 Cryst. (Me_2CO/Et_2O/petrol). Mp 117-119°. $[\alpha]_D^{20}$ +35 (c, 1.0 in $CHCl_3$).

N-*Benzoyl, 1,2,4,6-tetra-Ac:* [32795-21-4].
$C_{21}H_{25}NO_{10}$ M 451.4 Mp 150-153° (Et_2O/petrol). $[\alpha]_D^{20}$ +8 (c, 1.0 in $CHCl_3$).

Me glycoside: [14193-51-2]. *Methyl 3-amino-3-deoxy-α-D-mannopyranoside*
$C_7H_{15}NO_5$ M 193.1 Syrup.

Me glycoside, hydrochloride: [14133-35-8].
Cryst. Mp 205° dec. $[\alpha]_D$ +60 (H_2O).

Me glycoside, N-*Ac:* [14196-89-5].
$C_9H_{17}NO_6$ M 235.2 Cryst. (EtOH). Mp 241-243° (192-193°) dec. $[\alpha]_D$ +44 (c, 1.66 in H_2O).

Me glycoside, 3N,4,6-tri-Ac: [22412-70-0].
$C_{13}H_{21}NO_8$ M 319.3 Cryst. Mp 139-140°.

Me glycoside, 2,3N,4,6-tetra-Ac: [72523-35-4].
$C_{15}H_{23}NO_9$ M 361.3 Cryst. (Me_2CO/Et_2O). Mp 153° (142-143°). $[\alpha]_D$ +24.6 (c, 2.0 in $CHCl_3$), $[\alpha]_D$ +41 (c, 1.8 in H_2O), $[\alpha]_D$ +28 (c, 0.7 in H_2O).

Me glycoside, N-*benzoyl:* [22412-65-3].
$C_{14}H_{19}NO_6$ M 297.3 Amorph. solid.

Me glycoside, N-*benzoyl, 2,4,6-tri-Ac:* [22412-66-4].
$C_{20}H_{25}NO_9$ M 423.4 Needles (EtOH). Mp 144°.

Me glycoside, 4,6-O-benzylidene, N-*benzoyl:* [22412-67-5].
$C_{21}H_{23}NO_6$ M 385.4 Needles (EtOH). Mp 178-180°.

β-D-Pyranose-form

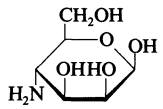
Me glycoside: Methyl 3-amino-3-deoxy-β-D-mannopyranoside
$C_7H_{15}NO_5$ M 193.1 Cryst. (as hydrochloride). Mp 230-231° dec. (hydrochloride). $[\alpha]_D$ −68.5 (H_2O).

1,6-Anhydro: [122204-79-9].
$C_6H_{11}NO_4$ M 161.1 Syrup.

1,6-Anhydro, hydrochloride: [122204-83-5].
Cryst. (EtOH). Mp 187° dec. $[\alpha]_D^{25}$ −102 (c, 0.7 in H_2O).

Baer, H.H. *et al, J.A.C.S.*, 1960, **82**, 3709 (α-*Me gly*)
Baer, H.H. *et al, Can. J. Chem.*, 1963, **41**, 1606 (β-*Me gly*)
Shigeharu, I. *et al, Chem. Pharm. Bull.*, 1966, **14**, 902, 1210; 1972, **20**, 2320 (*deriv, ms*)
Shibata, H. *et al, Agric. Biol. Chem.*, 1968, **32**, 1006 (α-*Me pyr N-benzoyl deriv, ir*)
Paulsen, H. *et al, Chem. Ber.*, 1971, **104**, 1311 (α-*pyr tetra-Ac,* α-*pyr penta-Ac*)
Jacobsen, S. *et al, Acta Chem. Scand., Ser. B*, 1988, **42**, 605 (β-*pyr deriv, pmr*)
Defaye, J., *Carbohydr. Res.*, 1991, **212**, 129 (α-*Me gly N-Ac, pmr*)

4-Amino-4-deoxymannose A-1-00107



β-D-Pyranose-*form*

$C_6H_{13}NO_5$ M 179.1

D-form [114912-49-1]
Syrup.

β-D-Pyranose-form

1,6-Anhydro:
$C_6H_{11}NO_4$ M 161.1 Cryst. (EtOH aq.) (as hydrochloride). Mp 175-180° dec. (hydrochloride). $[\alpha]_D^{18}$ −100.4 (c, 4.56 in H_2O).

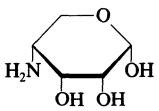
1,6-Anhydro, 2,3,4N-tri-Ac:
$C_{12}H_{17}NO_7$ M 287.2 Needles (EtOH). Mp 180°. $[\alpha]_D^{18}$ −76 (c, 0.54 in $CHCl_3$).

α-D-Furanose-form

Benzyl glycoside, 2,3-O-isopropylidene:
$C_{16}H_{23}NO_5$ M 309.3 Syrup.

James, S.P. *et al, J.C.S.*, 1946, 625 (β-D-pyr derivs)
Bashyal, B.P. *et al, Tetrahedron*, 1987, **43**, 3083 (α-D-fur deriv, pmr, ms)

4-Amino-4-deoxyribose A-1-00108



α-D-Pyranose-*form*

$C_5H_{11}NO_4$ M 149.1

α-D-Pyranose-form

Hydrochloride: [136766-50-2].
Syrup.

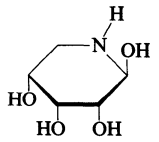
β-D-Pyranose-form

Hydrochloride: [136766-51-3].
Syrup.

Benzyl glycoside, 2,3-anhydro: [65518-85-6].
$C_{12}H_{15}NO_3$ M 221.2 Cryst. Mp 55°. $[\alpha]_D^{20}$ +54.4 ($CHCl_3$).

Kimmich, R. *et al, Annalen*, 1981, 1100 (*benzyl gly*)
Malik, A. *et al, Chem. Comm.*, 1984, 1530 (*benzyl gly*)
Witte, J.F. *et al, Tet. Lett.*, 1991, **32**, 3927 (*synth, pmr, cmr*)

5-Amino-5-deoxyribose A-1-00109



β-D-Pyranose-*form*

$C_5H_{11}NO_4$ M 149.1

D-form

Benzylphenylhydrazone, 5N-Ac: Cryst. ($MeOH/Et_2O$/petrol). Mp 143-144°. $[\alpha]_D^{23}$ −36.4 (c, 1.72 in MeOH).

β-D-Pyranose-form

3,4,5N-Tri-Ac:
$C_{11}H_{17}NO_7$ M 275.2 Cryst. (EtOAc). Mp 139-140°.

2,3,4,5N-Tetra-Ac:
$C_{13}H_{19}NO_8$ M 317.2 Cryst. (EtOAc). Mp 147-148°.

D-Furanose-form

N-*Ac:*
$C_7H_{13}NO_5$ M 191.1 Amorph. solid. $[\alpha]_D^{24}$ +19 (c, 1.6 in H_2O).

β-D-Furanose-form

Me glycoside, 2,3-O-isopropylidene: [14131-74-9].
$C_9H_{17}NO_4$ M 203.2 Oil. $[\alpha]_D^{25}$ −71.6 (c, 0.8 in $CHCl_3$).

Me glycoside, 2,3-O-isopropylidene, hydrochloride: Needles (EtOH). Mp 201.5-202°. $[\alpha]_D^{25}$ −34.5 (c, 6.3 in H_2O).

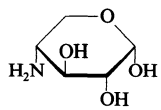
Benzyl glycoside, 2,3-O-isopropylidene, N-*Ac:*
$C_{17}H_{23}NO_5$ M 321.3 Cryst. (Et_2O/pentane). Mp 50°, Mp 65° (solvate).

DL-form

Di-Me acetal, 2,3,4,5N-tetra-Ac: [119830-25-0].
$C_{15}H_{25}NO_9$ M 363.3 Cryst. (EtOAc/cyclohexane). Mp 101-102°.

Hanessian, S. *et al, J.O.C.*, 1963, **28**, 2604 (D-fur deriv, ir, cryst struct)
Leonard, N.J. *et al, J. Het. Chem.*, 1966, **3**, 485 (*Me* β-D-fur deriv, pmr)
Defoin, A. *et al, Helv. Chim. Acta*, 1988, **71**, 1642 (DL-form, β-D-pyr deriv, ir, pmr, cmr)

4-Amino-4-deoxyxylose A-1-00110



α-D-Pyranose-*form*

$C_5H_{11}NO_4$ M 149.1

D-form

1,1-Diethyl dithioacetal, N-*benzoyl:* [91876-89-0].
$C_{16}H_{25}NO_4S_2$ M 359.5 Cryst. (MeOH/EtOAc/hexane). Mp 144-147°. $[\alpha]_D^{20}$ +15 (c, 0.9 in Pyr).

1,1-Diethyl dithioacetal, N-*benzoyl, 5-Ac:* [91876-88-9].
$C_{18}H_{27}NO_5S_2$ M 401.5 Cryst. (EtOAc/hexane). Mp 139-141°. $[\alpha]_D^{22}$ −10 (c, 2 in $CHCl_3$).

1,1-Diethyl dithioacetal, 5-benzoyl, N-*Ac:* [91876-87-8].
$C_{18}H_{27}NO_5S_2$ M 401.5 Cryst. (EtOAc/hexane). Mp 120-125°. $[\alpha]_D^{22}$ +27 (c, 2.5 in $CHCl_3$).

1,1-Diethyl dithioacetal, 4N,5-dibenzoyl: [91876-99-2].

$C_{23}H_{29}NO_5S_2$ M 463.6 Cryst. ($CHCl_3$/Et_2O). Mp 113-115°. $[\alpha]_D^{22}$ +21 (c, 1.4 in $CHCl_3$).

1,1-Diethyl dithioacetal, 2,3-O-isopropylidene, 4N,5-dibenzoyl: [91876-86-7].
$C_{26}H_{33}NO_5S_2$ M 503.6 Cryst. ($CHCl_3$/Et_2O). Mp 125-128°. $[\alpha]_D^{22}$ −41 (c, 1 in $CHCl_3$).

N,N-*Di-Me:*
$C_7H_{15}NO_4$ M 177.2 Cryst. (as hydrochloride). Mp 166-169° dec. (hydrochloride). $[\alpha]_D^{24}$ −18 (c, 2 in H_2O).

α-D-Pyranose-form

Me glycoside:
$C_6H_{13}NO_4$ M 163.1 Mp 196-197° dec. $[\alpha]_D$ +44 (c, 1 in H_2O).

Benzyl glycoside, 2,3-anhydro: Benzyl 2,3-anhydro-4-amino-4-deoxy-α-D-xylopyranoside
$C_{12}H_{15}NO_3$ M 221.2 Cryst. Mp 48-49°. $[\alpha]_D^{20}$ +91 ($CHCl_3$).

α-D-Furanose-form

1,2-O-Isopropylidene, N-*Ac:* [91876-94-7].
$C_{10}H_{17}NO_5$ M 231.2 Oil. $[\alpha]_D^{22}$ −92 (c, 0.3 in $CHCl_3$).

1,2-O-Isopropylidene, 5-benzoyl, N-*Ac:* [91876-95-8].
$C_{17}H_{21}NO_6$ M 335.3 Mp 135-137°. $[\alpha]_D^{22}$ −2 (c, 0.4 in $CHCl_3$).

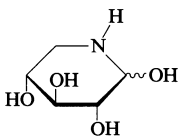
1,2:3,5-Di-O-isopropylidene, N-*benzoyl:* [91876-90-3].
$C_{18}H_{23}NO_5$ M 333.3 Cryst. Mp 106-110°. $[\alpha]_D^{22}$ −22 (c, 1.1 in $CHCl_3$).

β-L-Pyranose-form

Benzyl glycoside, 2,3-anhydro: Benzyl 2,3-anhydro-4-amino-4-deoxy-β-L-xylopyranoside
$C_{12}H_{15}NO_3$ M 221.2 Mp 37-38°. $[\alpha]_D^{20}$ +105 ($CHCl_3$).

Overend, W.G. *et al, Chem. Ind. (London),* 1963, 1840 (*Me* α-D-pyr)
Malik, A. *et al, Chem. Comm.,* 1984, 1530 (*benzyl gly, pmr*)
Coetzee, I. *et al, S. Afr. J. Chem.,* 1984, **37**, 11 (D-derivs, α-D-fur derivs, pmr, ms)

5-Amino-5-deoxyxylose A-1-00111



D-Pyranose-*form*

$C_5H_{11}NO_4$ M 149.1

D-form

5N-*Ac, benzylphenylhydrazone:* Cryst. (MeOH/Et_2O). Mp 132-133°. $[\alpha]_D^{23}$ 0 (c, 3.56 in MeOH).

D-Pyranose-form

N-*Ac:*
$C_7H_{13}NO_5$ M 191.1 Mp 163-164° (153-154°). $[\alpha]_D$ −21.8 (c, 2.69 in H_2O), $[\alpha]_D$ −11.3 (MeOH).

D-Furanose-form

N-*Ac:* Amorph. solid. $[\alpha]_D$ +13.2 (c, 1.36 in MeOH), $[\alpha]_D^{23}$ +30 (c, 0.6 in H_2O).

1,2,3,5N-Tetra-Ac:
$C_{13}H_{19}NO_8$ M 317.2 $[\alpha]_D^{20}$ +94 (c, 1.4 in MeOH).

α-D-Furanose-form

1,2-O-Isopropylidene: [4613-58-5].
$C_8H_{15}NO_4$ M 189.2 Mp 100-102°. $[\alpha]_D^{17}$ −12 (c, 2.6 in EtOH).

1,2-O-Isopropylidene, 3-benzyl: [59055-65-1].
$C_{15}H_{21}NO_4$ M 279.3 Syrup. $[\alpha]_D^{22}$ −70 ($CHCl_3$).

1,2-O-Isopropylidene, N-*Ac:*
$C_{10}H_{17}NO_5$ M 231.2 Rectangular plates. Mp 111-112°. $[\alpha]_D^{23}$ +31 (c, 2.29 in MeOH).

1,2-O-Isopropylidene, 3-Me: [59055-64-0].
$C_9H_{17}NO_4$ M 203.2 Syrup. $[\alpha]_D^{22}$ −70 ($CHCl_3$).

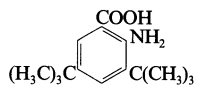
1,2-O-Cyclohexylidene, N-*Ac:*
$C_{13}H_{21}NO_5$ M 271.3 Mp 125-126°. $[\alpha]_D^{20}$ +39.2 (c, 1.0 in MeOH), $[\alpha]_D^{20}$ +18.2 (c, 1.0 in 0.1*M* HCl).

Akiya, S. *et al, Yakugaku Zasshi,* 1956, **76**, 1280 (α-D-fur deriv)
Paulsen, H. *et al, Annalen,* 1963, **670**, 121 (*fur deriv, ir*)
Jones, J.K.N. *et al, Can. J. Chem.,* 1963, **41**, 636 (*deriv*)
Jones, J.K.N. *et al, J.O.C.,* 1963, **28**, 2604 (*fur deriv, pyr deriv*)
Tronchet, J.M.J. *et al, Carbohydr. Res.,* 1981, **96**, 167 (α-D-fur deriv, pmr, ms)

2-Amino-3,5-di-*tert*-butylbenzoic acid A-1-00112

*2-Amino-3,5-bis(1,1-dimethylethyl)benzoic acid, 9CI. 3,5-Di-*tert*-butylanthranilic acid*

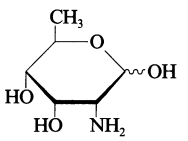
[26157-23-3]



$C_{15}H_{23}NO_2$ M 249.3
Mp 256-258°.

Franck, R.W. *et al, J.O.C.,* 1970, **35**, 3932.

2-Amino-2,6-dideoxyallose A-1-00113



D-Pyranose-*form*

$C_6H_{13}NO_4$ M 163.1

D-form [55385-63-2]

Hydrochloride: [51250-05-6].
Cryst. (Me_2CO/MeOH). Mp 135° dec. $[\alpha]_D^{20}$ +4 (c, 0.9 in H_2O).

N-*Ac:* [51250-01-2].
$C_8H_{15}NO_5$ M 205.2 Cryst. (EtOH). Mp 169-170°. $[\alpha]_D^{20}$ −88.5 (c, 0.4 in H_2O).

Brendel, K. *et al, Annalen,* 1966, **691**, 192 (*N-Ac*)
Perry, M.B. *et al, Carbohydr. Res.,* 1973, **31**, 131 (*synth*)

4-Amino-4,6-dideoxyallose A-1-00114

α-D-Pyranose-*form*

$C_6H_{13}NO_4$ M 163.1

D-form

N,N-*Di-Me:* [42213-97-8].
$C_8H_{17}NO_4$ M 191.2 Cryst. (EtOH/Et_2O) (as hydrochloride). Mp 166-168° (hydrochloride). $[\alpha]_D^{26}$ +38.09 → +33.2 (c, 1.52 in MeOH). CAS no. refers to hydrochloride.

α-D-Pyranose-form

Me glycoside: [37699-08-4]. *Methyl 4-amino-4,6-dideoxy-α-D-allopyranoside*
$C_7H_{15}NO_4$ M 177.2 Gum.

Me glycoside, N-*Ac:* [42214-19-7].
$C_9H_{17}NO_5$ M 219.2 Cryst. (MeOH/Et_2O). Mp 150-152°. $[\alpha]_D^{25}$ +235 (c, 0.75 in MeOH).

Me glycoside, 2,3-anhydro, N-*Ac:* [51255-03-9].
$C_9H_{15}NO_4$ M 201.2 Cryst. (EtOAc/petrol). Mp 186-187°. $[\alpha]_D$ +209 (c, 1 in $CHCl_3$).

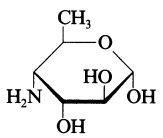
β-D-Pyranose-form

Me glycoside: [35942-00-8]. *Methyl 4-amino-4,6-dideoxy-β-D-allopyranoside*
$C_7H_{15}NO_4$ M 177.2 Cryst. (EtOH/Et_2O). Mp 174-176°. $[\alpha]_D^{26}$ −50.6 (c, 0.75 in MeOH). pK_a 7.20 (50% MeOH aq.).

Me glycoside, N-*Ac:* [35941-99-2].
Cryst. (EtOH/Et_2O). Mp 224-225°. $[\alpha]_D^{26}$ +3.9 (c, 0.4 in MeOH).

Bryant, C.P., *CA,* 1972, **76**, 86058d (D-form)
Stevens, C.L. *et al, Carbohydr. Res.,* 1972, **21**, 166 (*β-Me pyr deriv*)
Stevens, C.L. *et al, Methods Carbohydr. Chem.,* 1972, **6**, 235 (*α-Me pyr deriv*)
Stevens, C.L. *et al, J.O.C.,* 1973, **38**, 4311 (*α-Me-pyr deriv, β-Me pyr deriv, ir*)
Capek, K. *et al, Coll. Czech. Chem. Comm.,* 1987, **52**, 2248 (*anhydro, pmr*)

4-Amino-4,6-dideoxyaltrose A-1-00115



α-D-Pyranose-*form*

$C_6H_{13}NO_4$ M 163.1

D-form

N,N-*Di-Me:* [55570-42-8].
$C_8H_{17}NO_4$ M 191.2 Cryst. (2-propanol/Et_2O) (as hydrochloride). Mp 176-177° (hydrochloride). $[\alpha]_D^{25}$ +86.8 (c, 1 in H_2O). CAS no. refers to hydrochloride.

α-D-Pyranose-form

Me glycoside: [55637-43-9].
$C_7H_{15}NO_4$ M 177.2 Cryst. (propanol/Et_2O). Mp 116-117°. $[\alpha]_D^{24}$ +128.5 (c, 0.85 in MeOH).

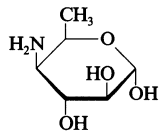
Me glycoside, N-*Ac:* [51255-06-2].
$C_9H_{17}NO_5$ M 219.2 Cryst. (2-propanol/Et_2O). Mp 151-153°. $[\alpha]_D^{22}$ +198.3 (c, 1 in MeOH).

Me glycoside, 2,3,4N-tri-Ac: [51269-16-0].
$C_{13}H_{21}NO_7$ M 303.3 Cryst. (2-propanol/pentane). Mp 168-169°. $[\alpha]_D^{24}$ +129.2 (c, 1 in $CHCl_3$).

Me glycoside, N,N-*di-Me:* [55570-40-6].
$C_9H_{19}NO_4$ M 205.2 Cryst. (Et_2O/petrol). Mp 110-112°. pK_a 7.52 (50% EtOH aq.).

Stevens, C.L. *et al, J.O.C.,* 1975, **40**, 2471 (D-deriv, α-Me pyr derivs, pmr)

4-Amino-4,6-dideoxyidose A-1-00116



$C_6H_{13}NO_4$ M 163.1

α-D-Pyranose-form

Me glycoside: [55637-42-8].
$C_7H_{15}NO_4$ M 177.2 Cryst. (EtOH/Et_2O/pentane). Mp 118-119°. $[\alpha]_D^{24}$ +82.2 (c, 0.6 in MeOH). pK_a 7.9 (50% MeOH aq.).

Me glycoside, N-*Ac:* [55570-18-8].
$C_9H_{17}NO_5$ M 219.2 Cryst. ($CHCl_3$/pentane). Mp 131-133°. $[\alpha]_D^{26}$ +155.8 (c, 1 in EtOH).

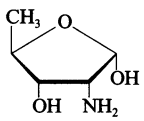
*Me glycoside, 2,3,4*N-*tri-Ac:* [55570-19-9].
$C_{13}H_{21}NO_7$ M 303.3 Cryst. (Me_2CO/pentane). Mp 97-98°. $[\alpha]_D^{26}$ +65.2 (c, 0.9 in MeOH).

Me glycoside, 2,3-dibenzyl, N-*Ac:* [55570-17-7].
$C_{23}H_{29}NO_5$ M 399.4 Cryst. (EtOH aq.). Mp 102-103°. $[\alpha]_D^{26}$ +20.8 (c, 1.18 in EtOH).

Me glycoside, N,N-*di-Me:* [55570-21-3].
$C_9H_{19}NO_4$ M 205.2 Cryst. (Me_2CO/pentane). Mp 86-87°. $[\alpha]_D^{29}$ +88.1 (c, 1.2 in $CHCl_3$). pK_a 7.19 (50% MeOH aq.).

Stevens, C.L. *et al, J.O.C.*, 1975, **40**, 2468 (*synth, Me gly derivs, pmr*)

2-Amino-2,5-dideoxyribose A-1-00117



$C_5H_{11}NO_3$ M 133.1

α-D-Furanose-form

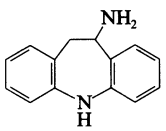
Benzyl glycoside, N-*benzoyl:* [119447-75-5].
$C_{19}H_{21}NO_4$ M 327.3 Gum.

Shiozaki, M. *et al, Agric. Biol. Chem.*, 1988, **52**, 2027 (*benzyl gly deriv, ir, pmr*)

10-Amino-10,11-dihydro-5*H*-dibenz[*b,f*]azepine A-1-00118

*10,11-Dihydro-5*H*-dibenz*[b,f]*azepin-10-amine, 9CI*

[30761-64-9]



$C_{14}H_{14}N_2$ M 210.2

(±)-form
Cryst. (hexane/C_6H_6). Mp 123°.

*5,10-Di-*N*-Me:* [21730-16-5]. ***Metapramine,*** *INN. 10,11-Dihydro-*N*,5-dimethyl-5*H*-dibenz*[b,f]*azepin-10-amine, 9CI. Rodostene. 19560 RP. Timaxel*
$C_{16}H_{18}N_2$ M 238.3 Antidepressant. Shows antinociceptive activity. Launched 1984. Mp 238-240° (as hydrochloride).

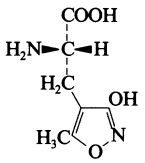
[93841-84-0, 103353-98-6]

South African Pat., 6 800 345, (1968) (*Rhône-Poulenc*); *CA*, **70**, 57689f (*synth, pharmacol*)
Ger. Pat., 2 159 678, (1972) (*Rhône-Poulenc*); *CA*, **77**, 88351p (*synth*)
Sommadossi, J.P. *et al, J. Chromatogr.*, 1982, **228**, 205 (*hplc*)
Decouvelaere, B. *et al, Therapie*, 1982, **37**, 249 (*metab*)
Sumirtapura, Y.C. *et al, Eur. J. Clin. Pharmacol.*, 1983, **25**, 673 (*pharmacol*)
Bougerolle, A.M. *et al, Eur. J. Drug Metab. Pharmacokinet.*, 1986, **11**, 113 (*pharmacokinet*)
Myers, C. *et al, Spectrosc. Lett.*, 1987, **20**, 945 (*pmr*)
Fialip, J. *et al, Life Sci.*, 1992, **50**, 161 (*pharmacol, exp*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 264.

α-Amino-2,3-dihydro-5-methyl-3-oxo-4-isoxazolepropanoic acid, 9CI A-1-00119

AMPA

[77521-29-0]



(S)-form

$C_7H_{10}N_2O_4$ M 186.1
Neurotransmitter which is bioisostere of glutamic acid; used to characterise neuroreceptors. AMPA-receptor agonist.

(R)-form [83654-13-1]
D-form
Cryst. (EtOH aq.). Mp >200°. $[\alpha]_D^{27}$ +19 (c, 0.18 in H_2O).

(S)-form [83643-88-3]
L-form
Cryst. (EtOH aq.). Mp >200°. $[\alpha]_D^{28}$ −21 (c, 0.19 in H_2O).

(±)-form [74341-63-2]
Cryst. + $1H_2O$ (H_2O). Mp 252° dec. (monohydrate).

Hydrobromide: [76010-07-6].
Cryst. (2-propanol). Mp 218-220° dec.

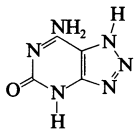
Et ester: [127020-32-0].
$C_9H_{14}N_2O_4$ M 214.2 Cryst. (H_2O). Mp 185-191° dec.

Honoré, T. *et al, Acta Chem. Scand., Ser. B*, 1980, **34**, 235 (*synth, cryst struct, pmr*)
Hansen, J.J. *et al, J.C.S. Perkin 1*, 1980, 1826 (*synth*)
Hansen, J.J. *et al, J. Med. Chem.*, 1983, **26**, 901 (*resoln, pmr*)
Begtrup, M. *et al, Synthesis*, 1993, 891 (*synth, cmr*)

7-Amino-1,4-dihydro-5*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-5-one, 9CI A-1-00120

*7-Amino-1*H*-v-triazolo[4,5-*d*]pyrimidin-5(4*H*)-one, 8CI. 6-Amino-2-oxo-8-azapurine. 8-Azaisoguanine*

[4730-46-5]



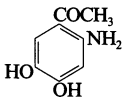
$C_4H_4N_6O$ M 152.1
Several tautomers possible. λ_{max} 277 nm (ε 2330) (pH 2); λ_{max} 250 (6310), 277 nm (9035) (pH 6.7).

Hydrochloride: Cryst. (6*M* HCl). Mp >320°.

Cavalieri, L.F. *et al, J.A.C.S.*, 1948, **70**, 3875; 1950, **72**, 2587 (*synth, uv*)
Blank, H.U. *et al, J.O.C.*, 1970, **35**, 1131 (*synth, uv*)
Melgunov, V.I., *J. Chromatogr.*, 1975, **109**, 204 (*detn*)
Montgomery, J.A. *et al, J. Med. Chem.*, 1983, **26**, 1483 (*synth, pmr, cmr, deriv*)

2′-Amino-4′,5′-dihydroxyacetophenone A-1-00121

4-Acetyl-5-amino-1,2-benzenediol



$C_8H_9NO_3$ M 167.1

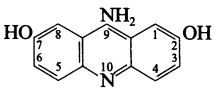
Di-Me ether: [4101-30-8]. *2′-Amino-4′,5′-dimethoxyacetophenone. 6-Aminoacetoveratrone*
$C_{10}H_{13}NO_3$ M 195.2 Golden needles (Et_2O). Mp 106-108°.

Simpson, J.C.E., *J.C.S.*, 1946, 95.

9-Amino-2,7-dihydroxyacridine A-1-00122

9-Amino-2,7-acridinediol, 9CI

[156644-27-8]



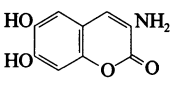
$C_{13}H_{10}N_2O_2$ M 226.2
Green solid. Mp >300°.

Vichet, A. *et al, J.O.C.*, 1994, **59**, 5156 (*synth, pmr*)

3-Amino-6,7-dihydroxy-2*H*-1-benzopyran-2-one, 9CI A-1-00123

3-Amino-6,7-dihydroxycoumarin

[22065-08-3]



$C_9H_7NO_4$ M 193.1
Shows hypotensive props. Mp 258-260°.

N-*Formyl:* [150624-46-7]. *3-(Formylamino)-6,7-dihydroxycoumarin.* ***Pseudoverdin***
$C_{10}H_7NO_5$ M 221.1 Prod. by *Pseudomonas aeruginosa*. Chromophore.

Di-Me ether: [150358-93-3]. *3-Amino-6,7-dimethoxy-2H-1-benzopyran-2-one. 3-Amino-6,7-dimethoxycoumarin*
$C_{11}H_{11}NO_4$ M 221.2 Cryst. (EtOH aq.). Mp 170°.

Di-Me ether, N-*formyl:* [150358-91-1].
$C_{12}H_{11}NO_5$ M 249.2 Mp 246°.

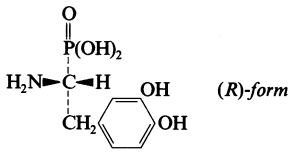
Di-Me ether, N-*Ac:* [150358-92-2]. *3-(Acetylamino)-6,7-dimethoxycoumarin*
$C_{13}H_{13}NO_5$ M 263.2 Cryst. (EtOH aq.). Mp 248°.

Fr. Pat., 1 523 317, (1968); *CA*, **72**, 31615v (*synth*)

Longerich, I. *et al*, *Z. Naturforsch., C*, 1993, **48**, 425 (*isol, synth, derivs*)

[1-Amino-2-(3,4-dihydroxyphenyl)ethyl] phosphonic acid, 9CI A-1-00124

[130848-98-5]



(*R*)-*form*

$C_8H_{12}NO_5P$ M 233.1

(*R*)-*form* [107439-34-9]
Phosphorus analogue of L-DOPA (see 2-Amino-3-(3,4-dihydroxyphenyl)propanoic acid, A-0-01830). Mp 254-255° dec. $[\alpha]_D^{20}$ −53 (c, 1 in 5*M* HCl) (100% op).

Salt with dibenzoyl-(−)-tartaric acid: Solid. Mp 164-165°. $[\alpha]_D^{20}$ −26 (c, 0.5 in MeOH).

(*S*)-*form* [107439-33-8]
Solid. Mp 240-250° dec. $[\alpha]_D^{20}$ +41 (c, 1 in 5*M* HCl) (80% op).

Salt with dibenzoyl-(+)-tartaric acid: Solid. Mp 173-174°. $[\alpha]_D^{20}$ −48 (c, 0.5 in MeOH).

3,4-Di-Me ether; di-Et ester: [104639-83-0]. Liq. $Bp_{0.1}$ 200°. $[\alpha]_D^{20}$ +12.10 (c, 2.15 in $CHCl_3$).

(±)-*form* [54627-43-9]
Solid. Mp 196°, Mp 265-266°.

3,4-Di-Me ether: [121245-51-0]. [*1-Amino-(3,4-dimethoxyphenyl)ethyl]phosphonic acid*
$C_{10}H_{16}NO_5P$ M 261.2 Plant growth regulator. Solid. Mp 259-260° dec.

3,4-Di-Me ether; di-Et ester: [107395-18-6]. *Diethyl [1-amino-(3,4-dimethoxyphenyl) ethyl]phosphonate*
$C_{14}H_{24}NO_5P$ M 317.3 Solid (as oxalate salt). Mp 126-127° (oxalate salt).

[104130-97-4, 107395-12-0, 107395-19-7, 107395-20-0, 107439-36-1]

Schöllkopf, U. *et al*, *Annalen*, 1987, 45 (*ester, ir, ms, pmr*)
Lejczak, B. *et al*, *Biochem. J.*, 1987, **242**, 81 (*synth, derivs, resoln, pmr, props*)
Kafarski, P. *et al*, *Pestic. Sci.*, 1989, **25**, 137 (*use*)
Maier, L., *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1990, **53**, 43 (*derivs, synth, pmr*)

Amino(dimethoxyphosphinyl) acetic acid A-1-00125

C-(*Dimethoxyphosphinyl)glycine*

$(MeO)_2P(O)CH(NH_2)COOH$

$C_4H_{10}NO_5P$ M 183.1

(±)-*form*
Me ester: [100945-13-9]. *Trimethyl aminophosphonoacetate*
$C_5H_{12}NO_5P$ M 197.1 Cryst. (MeOH). Mp 142-143°.

N-*Formyl, Me ester:*
$C_6H_{12}NO_6P$ M 225.1 Oil.

N-*Ac, Me ester:*
$C_7H_{14}NO_6P$ M 239.1 Cryst. (EtOAc/pentane). Mp 88-89°.

N-*Chloroacetyl, Me ester:*
$C_7H_{13}ClNO_6P$ M 273.6 Cryst. (EtOAc). Mp 105°.

N-tert-*Butoxycarbonyl:*
$C_9H_{18}NO_7P$ M 283.2 Solid. Mp 154-155°.

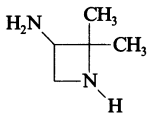
N-tert-*Butoxycarbonyl, Me ester:*
$C_{10}H_{20}NO_7P$ M 297.2 Cryst. (Et_2O/pentane). Mp 47-48°.

N-*Benzyloxycarbonyl, Me ester:*
$C_{13}H_{18}NO_7P$ M 331.2 Solid. Mp 80°.

Schmidt, U. *et al*, *Synthesis*, 1984, 53 (*synth, pmr*)
Horenstein, B.A. *et al*, *J.A.C.S.*, 1989, **111**, 6242 (*derivs, ms, ir, pmr*)
Daumas, M. *et al*, *Synth. Commun.*, 1990, **20**, 3395 (*synth, ms, pmr*)
Huang, N.Z. *et al*, *Tetrahedron*, 1990, **46**, 8067 (*pmr, use*)

3-Amino-2,2-dimethylazetidine A-1-00126

2,2-Dimethyl-3-azetidinamine, 9CI

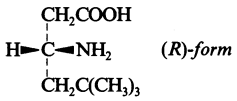


$C_5H_{12}N_2$ M 100.1

(±)-*form*
Dihydrochloride: [133891-84-6].
Solid. Mp 168-171°.

Frigola, J. *et al*, *J. Med. Chem.*, 1994, **37**, 4195 (*synth, ir*)

3-Amino-5,5-dimethylhexanoic acid, 9CI A-1-00127



(*R*)-*form*

$C_8H_{17}NO_2$ M 159.2

(*R*)-*form*
Hydrochloride: [158362-78-8].
Solid. Mp 190-192°. $[\alpha]_D^{25}$ −20.3 (c, 0.027 in H_2O).

(±)-*form*
Hydrochloride: [158414-70-1].
Solid. Mp 233-134°.
Et ester: [158362-81-3].
$C_{10}H_{21}NO_2$ M 187.2 Solid as hydrochloride. Mp 135-136°.
N-*Ac:* [158362-80-2].
$C_{10}H_{19}NO_3$ M 201.2 Oil.

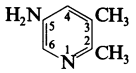
[158362-75-5, 158362-79-9]

Saeed, A. *et al*, *J. Med. Chem.*, 1994, **37**, 3247 (*synth, resoln, ir, pmr*)

5-Amino-2,3-dimethylpyridine A-1-00128

5,6-Dimethyl-3-pyridinamine, 9CI

[66093-07-0]



$C_7H_{10}N_2$ M 122.1
Cryst. ($CHCl_3$/hexane). Mp 75-76°.

Wai, J.S. *et al*, *J. Med. Chem.*, 1993, **36**, 249 (*synth, pmr*)

6-Amino-2,3-dimethylpyridine A-1-00129

5,6-Dimethyl-2-pyridinamine

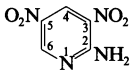
$C_7H_{10}N_2$ M 122.1
Solid. Mp 41-43°.

Tanga, M.J. *et al*, *J. Het. Chem.*, 1994, **31**, 1641 (*synth, pmr, cmr, uv*)

2-Amino-3,5-dinitropyridine A-1-00130

3,5-Dinitro-2-pyridinamine, 9CI

[3073-30-1]



$C_5H_4N_4O_4$ M 184.1
Yellow cryst. Mp 191-192°. pK_a 13.8 (as acid).

N-*Me:* [19404-40-1].
$C_6H_6N_4O_4$ M 198.1 Mp 163°.

N,N-*Di-Me:* [14585-26-3].
$C_7H_8N_4O_4$ M 212.1 Cryst. (EtOH). Mp 119°.

N,N-*Di-Et:*
$C_9H_{12}N_4O_4$ M 240.2 Mp 59°.

N-*Ph:* [18617-42-0].
$C_{11}H_8N_4O_4$ M 260.2 Mp 149°.

Harris, M.G. *et al*, *Can. J. Chem.*, 1977, **55**, 3800 (*synth, uv*)
de Bie, D.A. *et al*, *J.O.C.*, 1985, **50**, 484 (*synth, pmr, cmr*)
Woźniak, M. *et al*, *Annalen*, 1993, 7 (*synth, pmr*)

2-Amino-4,5-dinitropyridine A-1-00131

4,5-Dinitro-2-pyridinamine

[4487-53-0]

$C_5H_4N_4O_4$ M 184.1
Cryst. (Py aq.). Mp 217° dec.

Talik, T. *et al*, *Proc. Int. Symp. Nitro Compds.*, 1963, 81; *CA*, **64**, 2046f (*synth*)

4-Amino-3,5-dinitropyridine A-1-00132

3,5-Dinitro-4-pyridinamine, 9CI

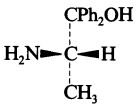
[31793-29-0]

$C_5H_4N_4O_4$ M 184.1

1-Oxide: [132683-65-9].
$C_5H_4N_4O_5$ M 200.1 Fine yellow cryst. (AcOH). Mp 210° dec.

Harris, M.G. *et al*, *Can. J. Chem.*, 1977, **55**, 3800 (*synth, uv*)
Woźniak, M. *et al*, *Annalen*, 1993, 7 (*pmr*)
Ritter, H. *et al*, *J. Het. Chem.*, 1995, **32**, 585 (*oxide*)

2-Amino-1,1-diphenyl-1-propanol A-1-00133



(*S*)-*form*

$C_{15}H_{17}NO$ M 227.3

(*S*)-*form*

Powder or needles (EtOH aq.). Mp 101.5-102.5°. $[\alpha]_D^{20}$ −85.9 (c, 2.77 in $CHCl_3$).

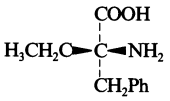
(±)-*form*

Powder. Mp 94-98°.

McKenzie, A. *et al*, *J.C.S.*, 1925, 283; 1926, 779 (*synth*)
Itsumo, S. *et al*, *J.C.S. Perkin 1*, 1985, 2039 (*synth*)
Weber, E. *et al*, *J.C.S. Perkin 2*, 1994, 1455 (*synth*)

2-Amino-2-ethyl-3-phenylpropanoic acid A-1-00134

α-Ethylphenylalanine, 9CI



(*R*)-*form*

$C_{11}H_{15}NO_2$ M 193.2

(*R*)-*form* [132616-90-1]

Mp >250°. $[\alpha]_D$ +25.4 (c, 1.0 in H_2O).

(*S*)-*form* [100665-68-7]

Powder. $[\alpha]_D$ −26.9 (c, 2.1 in H_2O).

N-*Ac:* [65484-34-6].
$C_{13}H_{17}NO_3$ M 235.2 Mp 223-225°. $[\alpha]_D^{21}$ +19.0 (c, 1.9 in MeOH).

Schöllkopf, U. *et al*, *Angew. Chem.*, 1978, **90**, 136 (*N-Ac*)
Kruizinga, W.H. *et al*, *J.O.C.*, 1988, **53**, 1826 (*resoln*)
U.S. Pat., 5 153 358, (1992); *CA*, **118**, 213538y (*S-form, synth, pmr, cmr*)
Studer, A. *et al*, *Annalen*, 1995, 217 (*R-form, synth, pmr, cmr, ms*)

(2-Aminoethyl)phosphinic acid, 9CI A-1-00135

[85618-16-2]

$H_2NCH_2CH_2PH(O)OH$

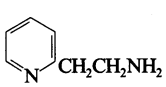
$C_2H_8NO_2P$ M 109.0
Solid. Mp 255°.

Dingwall, J.G. *et al*, *Tetrahedron*, 1989, **45**, 3785 (*synth, pmr, P-31 nmr*)

2-(2-Aminoethyl)pyridine, 8CI A-1-00136

2-Pyridineethanamine, 9CI

[2706-56-1]



$C_7H_{10}N_2$ M 122.1
Liq. d 1.02. Bp_{12} 92-93°. n_D^{20} 1.5360.

Dihydrochloride: [3343-39-3].
Cryst. Mp 189°.

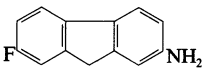
Dipicrate: [6628-61-1].
Yellow needles (EtOH). Mp 220°.

Westland, R.D. *et al*, *J.A.C.S.*, 1952, **74**, 6141 (*synth*)
Brady, E. *et al*, *J.O.C.*, 1961, **26**, 4757 (*synth*)

2-Amino-7-fluorofluorene A-1-00137

7-Fluoro-9H-fluoren-2-amine, 9CI

[363-16-6]



$C_{13}H_{10}FN$ M 199.2
Cryst. (EtOH aq.). Mp 135-136°. pK_a 3.53 (25°, 50% EtOH aq.).

N-*Ac:* [343-89-5].
$C_{15}H_{12}FNO$ M 241.2 Cryst. Mp 201-203°.

Miller, J.A. *et al*, *Cancer Res.*, 1955, **15**, 188 (*synth*)
Miller, J.A. *et al*, *J. Biol. Chem.*, 1959, **234** (*N-Ac*)
Grantham, P.H. *et al*, *J.O.C.*, 1961, **26**, 1008 (*pKa*)
Broyde, S. *et al*, *Chem. Biol. Interact.*, 1983, **47**, 69; *CA*, **100**, 204769a (*conformn*)

2-Amino-3-fluoro-2-(fluoromethyl)acetic acid A-1-00138

3-Fluoro-2-(fluoromethyl)alanine

$(FH_2C)_2C(NH_2)COOH$

$C_4H_7F_2NO_2$ M 139.1
Mp 182-183° dec.

Me ester: [154425-12-4].
$C_5H_9F_2NO_2$ M 153.1 Intracellular pH indicator. Syrup.

Me ester, hydrochloride: Mp 142-143°.

Bergmann, E.D. *et al*, *J.C.S.*, 1963, 3462 (*synth*)
Davis, F.A. *et al*, *Synthesis*, 1994, 701 (*Me ester, synth, pmr, cmr, F-19 nmr*)

3-Aminofuran A-1-00139

3-Furanamine, 9CI

[29212-69-9]

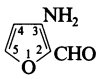
C_4H_5NO M 83.0
Stable in inert atmosphere or *in vacuo*. Polymerises rapidly on contact with air.

Prugh, J.D. *et al*, *J. Med. Chem.*, 1966, **9**, 254 (*synth*)

3-Amino-2-furancarboxaldehyde, 9CI A-1-00140

3-Amino-2-formylfuran

[56489-00-0]



$C_5H_5NO_2$ M 111.1
Cryst. (Et_2O) or oil. Mp 45-50°.

Gronowitz, S. *et al*, *Acta Chem. Scand., Ser. B*, 1975, **29**, 224 (*synth, ir, pmr*)

5-Amino-2-furancarboxaldehyde A-1-00141

2-Amino-5-formylfuran

[39116-21-7]

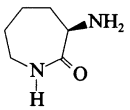
$C_5H_5NO_2$ M 111.1
Yellow solid. Polym. on heating.

Považanec, F. *et al*, *Chem. Pap.*, 1988, **42**, 677 (*synth, ir, pmr*)

3-Aminohexahydro-2*H*-azepin-2-one, 9CI A-1-00142

3-Amino-ε-caprolactam

[671-42-1]



(*R*)-*form*

$C_6H_{12}N_2O$ M 128.1

(*R*)-*form* [28957-33-7]

Hydrochloride: [26081-03-8].
Solid (MeOH). $[\alpha]_D^{26}$ +26.4 (c, 4 in 1*M* HCl) (>99% ee).

(*S*)-*form* [21568-87-6]

Mp 71-72°. $[\alpha]_D^{25}$ −34.0 (c, 4 in 1*M* HCl) (100% ee).

Hydrochloride: [26081-07-2].
Mp >270°. $[\alpha]_D^{25}$ −27.0 (c, 2.98 in 1*M* HCl).

(±)-*form* [17929-90-7]

Cryst. (EtOAc). Mp 68-71°, Mp 147-149°. $Bp_{0.1}$ 105°.

N-*Ac:*
$C_8H_{14}N_2O_2$ M 170.2 Cryst. (EtOAc). Mp 160-162°.

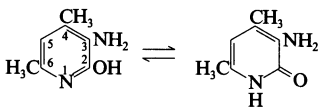
N-*Benzoyl:*
$C_{13}H_{16}N_2O_2$ M 232.2 Cryst. (EtOH). Mp 203-211°.

Pellegata, R. *et al*, *Synthesis*, 1978, 614 (*synth, S-form*)
Boyle, W.J. *et al*, *J.O.C.*, 1979, **44**, 4841 (*synth*)
Uchikawa, J. *et al*, *J. Het. Chem.*, 1994, **31**, 877 (*N-Ac, N-benzoyl*)

3-Amino-2-hydroxy-4,6-dimethylpyridine A-1-00143

3-Amino-4,6-dimethyl-2(1H)-pyridinone, 9CI.
3-Amino-4,6-dimethyl-2-pyridinol

[143708-29-6]



$C_7H_{10}N_2O$ M 138.1
Needles (H_2O). Mp 205°.

Collie, J.N. *et al*, *J.C.S.*, 1898, **73**, 229 (*synth*)
Saari, W.S. *et al*, *J. Med. Chem.*, 1992, **35**, 3792 (*synth, pmr*)
Gewald, K. *et al*, *Annalen*, 1995, 787 (*synth, pmr*)

3-Amino-6-hydroxy-2,4-dimethylpyridine A-1-00144

5-Amino-4,6-dimethyl-2(1H)-pyridinone, 9CI.
5-Amino-4,6-dimethyl-2-pyridinol

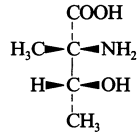
[39112-88-4]

$C_7H_{10}N_2O$ M 138.1
Needles (H_2O). Mp 221-222°.

Loth, H. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1972, **305**, 724 (*synth*)

2-Amino-3-hydroxy-2-methylbutanoic acid A-1-00145

α-Methylthreonine



(2*R*,3*R*)-*form*

$C_5H_{11}NO_3$ M 133.1

Props. given may refer to hydrochlorides (not stated but conc. HCl used in synth.).

(2R,3R)-form

D-allo-form

Mp 267-268° dec. $[\alpha]_D^{24}$ −13.0 (c, 0.3 in H_2O).

Me ester:

$C_6H_{13}NO_3$ M 147.1 Mp 159.5-160.5° (as hydrochloride). $[\alpha]_D^{20}$ −1.5 (c, 1.1 in H_2O).

(2R,3S)-form

D-form

Mp 211-213°. $[\alpha]_D^{25}$ +13.0 (c, 0.95 in H_2O).

(2S,3R)-form

L-form

Mp 214-219°. $[\alpha]_D^{20}$ −14.1 (c, 1.08 in H_2O).

(2S,3S)-form

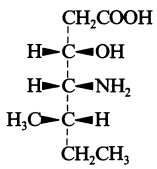
L-allo-form

Mp 265-267° dec. $[\alpha]_D^{21}$ −12.6 (c, 0.98 in H_2O).

Seebach, D. *et al*, *Helv. Chim. Acta*, 1987, **70**, 1194 (*synth, ir, pmr, cmr, ms*)

Moon, S.H. *et al*, *J.A.C.S.*, 1994, **116**, 7405 (*synth*)

4-Amino-3-hydroxy-5-methylheptanoic acid A-1-00146



$C_8H_{17}NO_3$ M 175.2

(3S,4R,5S)-form

Isostatine

Component of Didemnin A.

N-tert-*Butyloxycarbonyl:* Semisolid. $[\alpha]_D$ −8.7 (c, 2.4 in $CHCl_3$).

N-tert-*Butyloxycarbonyl, Me ester:* Oil. $[\alpha]_D$ −1.5 (c, 1.17 in $CHCl_3$).

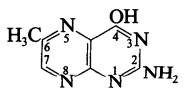
[114607-51-1, 116261-18-8]

Lloyd-Williams, P. *et al*, *J.C.S. Perkin 1*, 1994, 1969 (*synth, bibl*)

2-Amino-4-hydroxy-6-methylpteridine A-1-00147

2-Amino-6-methyl-4(1H)-pteridinone, 9CI. 2-Amino-6-methyl-4-pteridinol. 6-Methylpterin

[708-75-8]



$C_7H_7N_5O$ M 177.1

At least two NH tautomers possible. Bright yellow cryst. Mp >300°.

N^8-*Oxide:* [20210-03-1].

$C_7H_7N_5O_2$ M 193.1 Cryst. Mp >320°.

N^2-*Ac:* [19962-30-2].

$C_9H_9N_5O_2$ M 219.2 Cryst. Mp 315-320° dec.

[13165-98-5]

Boon, W.R. *et al*, *J.C.S.*, 1951, 1497 (*synth*)

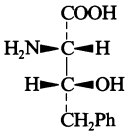
Taylor, E.C. *et al*, *J.A.C.S.*, 1973, **95**, 6407 (*synth*)

Waring, P. *et al*, *Aust. J. Chem.*, 1985, **38**, 629 (*synth*)

Tobias, S. *et al*, *Chem. Ber.*, 1985, **118**, 354 (*cmr*)

2-Amino-3-hydroxy-4-phenylbutanoic acid A-1-00148

α-Amino-β-hydroxybenzenebutanoic acid, 9CI



$C_{10}H_{13}NO_3$ M 195.2

(2S,3R)-form [157543-53-8]

Powder. Mp 135-138°.

Pu, Y. *et al*, *J.O.C.*, 1994, **59**, 3642 (*synth, ir, pmr, ms*)

3-Amino-1-hydroxy-1,1-propanediphosphonic acid A-1-00149

(3-Amino-1-hydroxypropylidene)bis[phosphonic acid], 9CI. ***Pamidronic acid, BAN, INN.*** *Aminomux. Aredia. CGP 23339. APD*

[40391-99-9]

$H_2NCH_2CH_2C(OH)[P(O)(OH)_2]_2$

$C_3H_{11}NO_7P_2$ M 235.0

Suppresses bone resorption. Used in treatment of Paget's disease and malignant hypercalcaemia. Launched 1989. Mp 237-238°.

▶ Exp. nephrotoxic effects.

Di-Na salt: [57248-88-1]. ***Pamidronate disodium, USAN***

Solid + $5H_2O$.

▶ Exp. fetotoxic and other reprod. effects. SZ6525000.

Frijlink, W.B. *et al*, *Lancet*, 1979, **i**, 799, 803 (*pharmacol*)

Worms, K.H. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **457**, 214 (*synth*)

Bijvoet, O.L. *et al*, *Int. Congr. Ser. Excerpta Med.*, 1980, **511**, 132 (*rev*)

Shinoda, H. *et al*, *Calcif. Tissue Int.*, 1983, **35**, 87 (*pharmacol*)

Wingen, F. *et al*, *Arzneim.-Forsch.*, 1987, **37**, 1037 (*pharmacokinet*)

Bisphosphonates and Tumor Osteolysis, (Eds. Brunner, K.W., *et al*), Springer-Verlag, Berlin, 1989 (*book*)

Flesch, G. *et al*, *J. Chromatogr.*, 1989, **489**, 446 (*hplc*)

Gallacher, S.J. *et al*, *Lancet*, 1989, **ii**, 42 (*side effects*)

Hoggarth, C.R. *et al*, *Anal. Proc. (London)*, 1990, **27**, 18 (*hplc*)

Cal, J.-C. *et al*, *Toxicology*, 1990, **65**, 179 (*pharmacokinet, tox*)

Fitton, A. *et al*, *Drugs*, 1991, **41**, 289 (*rev*)

Flesch, G. *et al*, *J. Chromatogr.*, 1991, **568**, 261 (*hplc*)

Kellihan, M.J. *et al*, *Ann. Pharmacother.*, 1992, **10**, 1262, 1310 (*rev*)

Graepel, P. *et al*, *Arzneim.-Forsch.*, 1992, **42**, 654 (*reprod, tox*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 660.

(1-Amino-2-hydroxypropyl) phosphinic acid A-1-00150

[95691-17-1]

$H_3CCH(OH)CH(NH_2)PH(O)OH$

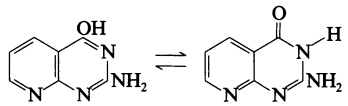
$C_3H_{10}NO_3P$ M 139.0

Isostere of threonine (see 2-Amino-3-hydroxybutanoic acid, A-0-02271). Microcryst. V. sol. H_2O. Mp 218-220° dec.

Bayliss, E.K. *et al*, *J.C.S. Perkin 1*, 1984, 2845 (*synth, ir, tlc, pmr, P-31 nmr*)

2-Amino-4-hydroxypyrido[2,3-*d*]pyrimidine A-1-00151

*2-Aminopyrido[2,3-*d*]pyrimidin-4(3H)-one. 2-Aminopyrido[2,3-*d*]pyrimidin-4-ol. 5-Deazapterin*



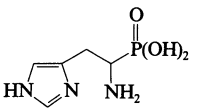
$C_7H_6N_4O$ M 162.1

Hydrochloride: V. pale pink solid.

Ivery, M.T.G. *et al*, *J. Het. Chem.*, 1994, **31**, 1385 (*synth, uv, pmr*)

[1-Amino-2-(4-imidazolyl) ethyl]phosphonic acid A-1-00152

Phosphonohistidine



$C_5H_{10}N_3O_3P$ M 191.1

(±)-***form*** [156721-55-0]

Cryst. + $2H_2O$ (H_2O). Mp 255-256°. pK_{a1} 2.9, pK_{a2} 4.9, pK_{a3} 6.9, pK_{a4} 9.8.

N-*Benzyl:*

$C_{12}H_{16}N_3O_3P$ M 281.2 Cryst. (H_2O). Mp 258.5-260° dec.

N-*Benzyl, di-Et ester:*

$C_{16}H_{24}N_3O_3P$ M 337.3 Syrup.

Merrett, J.H. *et al*, *J.C.S. Perkin 1*, 1988, 61 (*synth, pmr, props*)

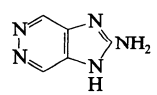
Kharmatov, A.B., *Bioorg. Khim.*, 1990, **16**, 1290; *Sov. J. Bioorg. Chem. (Engl. Transl.)*, 1990, **16**, 733 (*synth, pmr, tlc*)

Wu, Y.L. *et al*, *Chin. Chem. Lett.*, 1991, **2**, 95 (*synth, pmr*)

2-Aminoimidazo[4,5-*d*] pyridazine A-1-00153

*1H-Imidazo[4,5-*d*]pyridazin-2-amine, 9CI.* ***Zarzissine***

[160568-14-9]



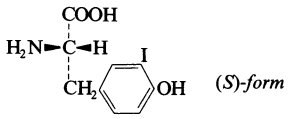
$C_5H_5N_5$ M 135.1

Alkaloid from the Mediterranean sponge *Anchinoe paupertas*. Cytotoxic. Powder. Subl. 270-271°.

Bouaicha, N. *et al, J. Nat. Prod.*, 1994, **57**, 1455 (*isol, uv, ir, pmr, cmr, ms, struct*)

2-Amino-3-(3-iodo-4-hydroxyphenyl)propanoic acid A-1-00154

3-Iodotyrosine, 9CI. Monoiodotyrosine. Iotyrosine



(*S*)-*form*

$C_9H_{10}INO_3$ M 307.0

^{131}I labelled cpd. is used as a radioactive agent.

(*S*)-*form* [70-78-0]

L-form

Occurs in thyroid tissue and human blood serum. Prod. by sponges. Cryst. (H_2O). Sol. hot H_2O. Mp 202-204°. $[\alpha]_D^{20}$ −4.4 (c, 5 in 1*M* HCl).

(±)-*form*

Cryst. + $1H_2O$ (H_2O). Mp 200-201° dec.

[16624-40-1, 19254-01-4, 20520-42-7, 60345-92-8, 70277-02-0, 78758-99-3]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 1189B (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 256C (*ir*)

Harington, C.R. *et al, Biochem. J.*, 1944, **38**, 320 (*synth*)

Pitt-Rivers, R. *et al, Chem. Ind. (London)*, 1956, 21 (*synth*)

Hillman, G. *et al, Hoppe Seyler's Z. Physiol. Chem.*, 1956, **305**, 177 (*synth*)

Wynn, J., *Arch. Biochem. Biophys.*, 1960, **88**, 98.

Bednar, J. *et al, Radiochem. Radioanal. Lett.*, 1980, **45**, 377 (*use*)

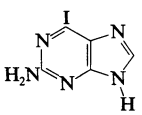
Baron, M.H. *et al, J. Chim. Phys. Phys.-Chim. Biol.*, 1983, **80**, 729 (*Raman*)

Okabe, N. *et al, Acta Cryst. C*, 1995, **51**, 1700 (*cryst struct*)

2-Amino-6-iodopurine A-1-00155

6-Iodo-9H-purin-2-amine, 9CI

[19690-23-4]



$C_5H_4IN_5$ M 261.0

Solid. Mp 240° dec.

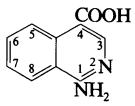
Tetrabutylammonium salt: Cryst. (EtOAc). Mp 114-116°.

Benzyltriethylammonium salt: Solid. Mp 156-159° (effervescence).

Koda, R.T. *et al, J. Pharm. Sci.*, 1968, **57**, 2056 (*synth, uv*)

Bisacchi, G.S. *et al, J.O.C.*, 1995, **60**, 2902 (*synth*)

1-Amino-4-isoquinolinecarboxylic acid A-1-00156



$C_{10}H_8N_2O_2$ M 188.1

Cryst. (H_2O). Mp 249-250°.

Bergstrom, F.W. *et al, J.A.C.S.*, 1940, **62**, 3030 (*synth*)

3-Amino-4-isoquinolinecarboxylic acid A-1-00157

$C_{10}H_8N_2O_2$ M 188.1

Et ester:

$C_{12}H_{12}N_2O_2$ M 216.2 Yellow needles. Mp 116-117°.

Nitrile: [68531-68-0]. *3-Amino-4-cyanoisoquinoline*

$C_{10}H_7N_3$ M 169.1 Pale yellow needles. Mp 171-172°.

Kikuchi, K. *et al, Chem. Lett.*, 1978, 677 (*nitrile*)

Suzuki, H. *et al, Synthesis*, 1995, 763 (*nitrile, Et ester*)

5-Amino-4-isoquinolinecarboxylic acid A-1-00158

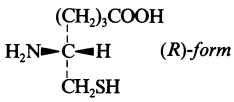
[62781-93-5]

$C_{10}H_8N_2O_2$ M 188.1

Yellow cryst. Mp 232°.

Ger. Pat., 2 631 661, (1977); *CA*, **86**, 189905p (*synth*)

5-Amino-6-mercaptohexanoic acid, 9CI A-1-00159



(*R*)-*form*

$C_6H_{13}NO_2S$ M 163.2

(*R*)-*form*

L-form

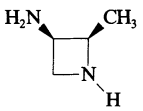
Hydrochloride: [162954-86-1]. Cryst. Mp 115-116°. $[\alpha]_D^{22}$ −17.3 (c, 1.04 in H_2O).

[162954-85-0]

Chauvel, E.N. *et al, J. Med. Chem.*, 1994, **37**, 2950 (*synth, pmr*)

3-Amino-2-methylazetidine A-1-00160

2-Methyl-3-azetidinamine, 9CI



(2*RS*,3*RS*)-*form*

$C_4H_{10}N_2$ M 86.1

(*2RS,3RS*)-*form*

(±)-cis-*form*

Dihydrochloride: [133891-81-3]. Solid. Mp 181-183°.

(*2RS,3SR*)-*form*

(±)-trans-*form*

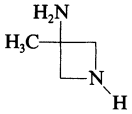
Dihydrochloride: [133224-78-9]. Solid. Mp 165-168°.

Frigola, J. *et al, J. Med. Chem.*, 1994, **37**, 4195 (*synth, ir, pmr*)

3-Amino-3-methylazetidine A-1-00161

3-Methyl-3-azetidinamine, 9CI

[147293-71-8]



$C_4H_{10}N_2$ M 86.1

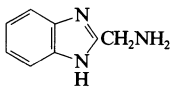
Hydrochloride (1:2): [124668-47-9]. Mp 196-199°.

Frigola, J. *et al, J. Med. Chem.*, 1993, **36**, 801 (*synth, ir*)

2-(Aminomethyl) benzimidazole A-1-00162

1H-Benzimidazole-2-methanamine

[5805-57-2]



$C_8H_9N_3$ M 147.1

Mp 48-51°.

Monohydrochloride: [7757-21-3]. Mp 227-229°.

Dihydrochloride: [5993-91-9]. Needles (EtOAc). Mp 268-270° dec.

[5993-91-9]

Cescon, L.A. *et al, J.O.C.*, 1962, **27**, 581 (*synth, ir*)

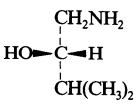
Kanaoka, Y. *et al, Chem. Pharm. Bull.*, 1969, **17**, 2381 (*synth, uv*)

Aminabhavi, T.M. *et al, Inorg. Chim. Acta*, 1986, **125**, 125.

Reddy, B.S. *et al, J. Indian Chem. Soc.*, 1988, **65**, 853 (*synth, ir, pmr, ms*)

1-Amino-3-methyl-2-butanol, 9CI A-1-00163

[17687-58-0]



(*S*)-*form*

$C_5H_{13}NO$ M 103.1

(*S*)-*form* [160168-49-0]

$[\alpha]_D^{20}$ +17.3 (c, 1 in MeOH) (97.2% ee).

(±)-*form* [123934-11-2]

Cryst. Mp 27°. Bp_{754} 174°.

Hydrochloride: Cryst. (EtOH). Mp 110°.

Krasuskii, K.A. *et al, CA*, 1930, **24**, 1082 (*synth*)

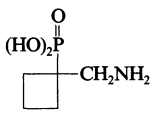
Kjaer, A. *et al, Acta Chem. Scand.*, 1962, **16**, 591 (*synth*)

Koppenhoefer, B. *et al, Synthesis*, 1994, 1141 (*S-form, synth, pmr, cmr*)

1-(Aminomethyl) cyclobutanephosphonic acid A-1-00164

1-(Aminomethyl)-1-cyclobutylphosphonic acid, 9CI

[135603-62-2]



$C_5H_{12}NO_3P$ M 165.1
Solid. Mp >260°.

Di-Et ester: [135603-30-4]. *Diethyl [1-(aminomethyl)-1-cyclobutyl]phosphonate* $C_9H_{20}NO_3P$ M 221.2 Liq. $Bp_{0.5}$ 86°.

Diisopropyl ester: [135603-31-5]. *Diisopropyl [1-(aminomethyl)-1-cyclobutyl]phosphonate* $C_{11}H_{24}NO_3P$ M 249.2 Liq. $Bp_{0.5}$ 98°.

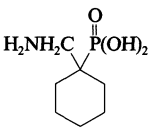
Dibutyl ester: [135603-32-6]. *Dibutyl [1-(aminomethyl)-1-cyclobutyl]phosphonate* $C_{13}H_{28}NO_3P$ M 277.3 Liq. $Bp_{0.4}$ 118°.

Nasser, J. *et al, Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **55**, 137 (*synth, pmr, P-31 nmr*)

1-(Aminomethyl) cyclohexanephosphonic acid A-1-00165

1-(Aminomethyl)-1-cyclohexylphosphonic acid, 9CI

[135603-64-4]



$C_7H_{16}NO_3P$ M 193.1
Solid. Mp >260°.

Di-Et ether: [135603-36-0]. *Diethyl [1-(aminomethyl)-1-cyclohexyl]phosphonate* $C_{11}H_{24}NO_3P$ M 249.2 Liq. $Bp_{0.5}$ 95°.

Diisopropyl ester: [135603-37-1]. *Diisopropyl [1-(aminomethyl)-1-cyclohexyl]phosphonate* $C_{13}H_{28}NO_3P$ M 277.3 Liq. $Bp_{0.5}$ 105°.

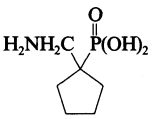
Dibutyl ester: [135603-38-2]. *Dibutyl [1-(aminomethyl)-1-cyclohexyl]phosphonate* $C_{15}H_{32}NO_3P$ M 305.3 Liq. $Bp_{0.2}$ 140°.

Nasser, J. *et al, Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **55**, 137 (*synth, pmr, P-31 nmr*)

1-(Aminomethyl) cyclopentanephosphonic acid A-1-00166

1-(Aminomethyl)-1-cyclopentylphosphonic acid, 9CI

[135603-63-3]



$C_6H_{14}NO_3P$ M 179.1
Solid. Mp >260°.

Di-Et ester: [135603-33-7]. *Diethyl [1-(aminomethyl)-1-cyclopentyl]phosphonate* $C_{10}H_{22}NO_3P$ M 235.2 Liq. $Bp_{0.5}$ 90°.

Diisopropyl ester: [135603-34-8]. *Diisopropyl [1-(aminomethyl)-1-cyclopentyl]phosphonate* $C_{12}H_{26}NO_3P$ M 263.3 Liq. $Bp_{0.5}$ 100°.

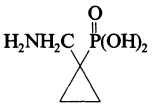
Dibutyl ester: [135603-35-9]. *Dibutyl [1-(aminomethyl)-1-cyclopentyl]phosphonate* $C_{14}H_{30}NO_3P$ M 291.3 Liq. $Bp_{0.5}$ 132°.

Nasser, J. *et al, Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **55**, 137 (*synth, pmr, P-31 nmr*)

1-(Aminomethyl) cyclopropanephosphonic acid A-1-00167

1-(Aminomethyl)-1-cyclopropylphosphonic acid, 9CI

[135603-61-1]



$C_4H_{10}NO_3P$ M 151.1
Solid. Mp >260°.

Di-Et ester: [135603-27-9]. *Diethyl [1-(aminomethyl)-1-cyclopropyl]phosphonate* $C_8H_{18}NO_3P$ M 207.2 Liq. $Bp_{0.5}$ 83°.

Diisopropyl ester: [135603-28-0]. *Diisopropyl [1-(aminomethyl)-1-cyclopropyl]phosphonate* $C_{10}H_{22}NO_3P$ M 235.2 Liq. $Bp_{0.5}$ 96°.

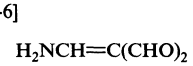
Dibutyl ester: [135603-29-1]. *Dibutyl [1-(aminomethyl)-1-cyclopropyl]phosphonate* $C_{12}H_{26}NO_3P$ M 263.3 Liq. $Bp_{0.5}$ 110°.

Nasser, J. *et al, Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **55**, 137 (*synth, pmr, P-31 nmr*)

(Aminomethylene)propanedial, 9CI A-1-00168

2,2-Diformylethenamine. 2-Amino-1,1-ethylenedicarboxaldehyde

[135304-92-6]



$C_4H_5NO_2$ M 99.0
Cryst. (C_6H_6). Mp 124-125°.

N-*Me:* [160651-00-3].
$C_5H_7NO_2$ M 113.1 Cryst. (cyclohexane). Mp 110°.

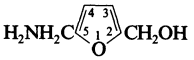
N,N-*Di-Me:* [73312-68-2].
$C_6H_9NO_2$ M 127.1 Mp 41-42°.

Takagi, K. *et al, J. Het. Chem.*, 1994, **31**, 973.

5-(Aminomethyl)-2-furanmethanol, 9CI A-1-00169

2-(Aminomethyl)-5-(hydroxymethyl)furan. 5-(Hydroxymethyl)furfurylamine

[88910-22-9]

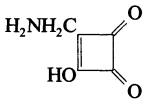


$C_6H_9NO_2$ M 127.1
Liq.

Holfinger, M.S. *et al, J.O.C.*, 1995, **60**, 1595 (*synth, ir, pmr, cmr, ms*)

3-(Aminomethyl)-4-hydroxy-3-cyclobutene-1,2-dione, 9CI A-1-00170

[162331-75-1]

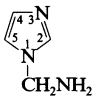


$C_5H_5NO_3$ M 127.0
Solid. Mp 124-168° dec.

Campbell, E.F. *et al, J.O.C.*, 1995, **60**, 1470 (*synth, pmr, ir*)

1-(Aminomethyl)imidazole A-1-00171

1H-Imidazole-1-methanamine



$C_4H_7N_3$ M 97.1

N-*Benzoyl:* [41951-40-0]. N-(*1H-Imidazol-1-ylmethyl)benzamide, 9CI*
$C_{11}H_{11}N_3O$ M 201.2 Mp 152-154°.

N,N-*Di-Me:* [23230-39-9]. *1-(Dimethylaminomethyl)imidazole*
$C_6H_{11}N_3$ M 125.1 Oil. Bp_2 100-102°.

Katritzky, A.R. *et al, J.O.C.*, 1988, **53**, 5685 (*N,N-di-Me*)

Pernak, J. *et al, Synthesis*, 1994, 1405 (*N-benzoyl*)

2-(Aminomethyl)imidazole A-1-00172

1H-Imidazole-2-methanamine, 9CI

[53332-80-2]

$C_4H_7N_3$ M 97.1

Hydrochloride (1:2): [22600-77-7]. Cryst. (MeOH/Et_2O or 2-propanol aq.). Mp 256-258° (240-242°).

N,N-*Di-Me:* [54534-78-0].
$C_6H_{11}N_3$ M 125.1 Cryst. Mp 63-65°.

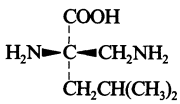
Gebert, U. *et al, Annalen*, 1968, **718**, 249 (*synth, pmr*)

Godefroi, E.F. *et al, J.O.C.*, 1978, **43**, 1603 (*synth*)

Schunack, W. *et al, J. Het. Chem.*, 1984, **21**, 753 (*synth*)

2-(Aminomethyl)leucine, 9CI A-1-00173

2-Amino-2-(aminomethyl)-4-methylpentanoic acid. Aml



(*R*)-*form*

$C_7H_{16}N_2O_2$ M 160.2

(***R*)-*form*** [170384-28-8]
L-form
Powder. Mp >220° dec. $[\alpha]_D$ +32.0 (c, 0.2 in H_2O).

(***S*)-*form*** [170384-27-7]
D-form
Powder. Mp >226° dec. $[\alpha]_D$ −25.2 (c, 0.2 in H_2O).

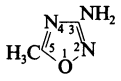
(±)-***form*** [170384-24-4]
DL-form
Powder. Mp 224.5-226.5°.

Obrecht, D. *et al, Helv. Chim. Acta*, 1995, **78**, 703 (*synth, ir, pmr, abs config*)

3-Amino-5-methyl-1,2,4-oxadiazole A-1-00174

5-Methyl-1,2,4-oxadiazol-3-amine, 9CI

[40483-47-4]



$C_3H_5N_3O$ M 99.0
Cryst. (C_6H_6 or toluene). Mp 117-119°.

N-*Me:*
$C_4H_7N_3O$ M 113.1 Mp 75-76°.

Anderson, G.W. *et al, J.A.C.S.*, 1942, **64**, 2902 (*synth*)
Buscemi, S. *et al, Synthesis*, 1995, 917 (*synth*)

5-Amino-3-methyl-1,2,4-oxadiazole A-1-00175

[3663-39-6]

$C_3H_5N_3O$ M 99.0
Needles (H_2O). Mp 159-160.5°.

Huffman, K.R. *et al, J.O.C.*, 1963, **28**, 1816 (*synth*)
Eloy, F. *et al, Helv. Chim. Acta*, 1966, **49**, 1430 (*synth*)
Cariati, F. *et al, Spectrochim. Acta A*, 1980, **36**, 1029 (*ir*)

4-Amino-4-methylpentanoic acid, 9CI A-1-00176

[3235-46-9]

$(H_3C)_2C(NH_2)CH_2CH_2COOH$

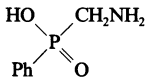
$C_6H_{13}NO_2$ M 131.1
Cryst. (MeOH/Et_2O). Mp 140°, Mp 268-269°.

Hydrochloride: [62000-69-5].
Cryst. (MeOH/Et_2O). Mp 178-179°.

Schumann, E.L. *et al, J. Med. Pharm. Chem.*, 1962, **5**, 464 (*synth*)
Baird, M.S. *et al, Synthesis*, 1994, 1471 (*synth*)

(Aminomethyl) phenylphosphinic acid A-1-00177

[15901-08-3]



$C_7H_{10}NO_2P$ M 171.1
Solid. Mp 286-287°.

[97611-02-4, 145932-38-3, 145932-39-4]

Popoff, I.C. *et al, J.O.C.*, 1963, **28**, 2898 (*synth, derivs, ir*)

1-Amino-2-methyl-2-propanethiol, 9CI A-1-00178

1-Amino-2-mercapto-2-methylpropane

[7684-18-6]

$(H_3C)_2C(SH)CH_2NH_2$

$C_4H_{11}NS$ M 105.2

Hydrochloride: [32047-53-3].
Solid (EtOH/EtOAc). Mp 202-203°.

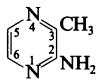
N-*Ac:* [89584-09-8].
$C_6H_{13}NOS$ M 147.2 No phys. props. descr.

Crooks, H.M. *et al, CA*, 1950, **44**, 9439d (*synth*)
Roy, B. *et al, J.O.C.*, 1994, **59**, 7019 (*synth, pmr, ir, cmr*)

2-Amino-3-methylpyrazine, 8CI A-1-00179

3-Methylpyrazinamine, 9CI

[19838-08-5]



$C_5H_7N_3$ M 109.1
Needles (hexane/EtOAc). Mp 174° (169-171°).

1-Oxide: [103965-75-9].
$C_5H_7N_3O$ M 125.1 Solid (MeOH). Mp 205-207°.

4-Oxide: [103965-76-0].
$C_5H_7N_3O$ M 125.1 Mp 175-177°. Sublimes.

Gainer, H. *et al, J.O.C.*, 1961, **26**, 2360 (*synth*)
Cox, R.H. *et al, J. Phys. Chem.*, 1968, **72**, 1642 (*pmr*)
Sato, N. *et al, J. Het. Chem.*, 1980, **17**, 142; 1985, **22**, 1145 (*synth, oxides*)
Sato, N. *et al, Synthesis*, 1994, 931 (*synth, pmr, ir*)

2-Amino-5-methylpyrazine, 8CI A-1-00180

5-Methylpyrazinamine, 9CI

[5521-58-4]

$C_5H_7N_3$ M 109.1
Needles (C_6H_6). Mp 120-121° (116°).

N-*Ac:*
$C_7H_9N_3O$ M 151.1 Mp 211-212°. Sublimes above 195°.

1-Oxide: [28082-77-1].
$C_5H_7N_3O$ M 125.1 Solid (EtOAc/EtOH). Mp 221-223°.

4-Oxide: [103965-77-1].
$C_5H_7N_3O$ M 125.1 Needles (EtOAc). Mp 213-214°.

Weijlard, J. *et al, J.A.C.S.*, 1945, **67**, 802 (*synth*)
Pitré, D. *et al, Chem. Ber.*, 1966, **99**, 364; 1967, **100**, 560 (*synth, uv*)
Sato, N. *et al, J. Het. Chem.*, 1980, **17**, 142; 1985, **22**, 1145; 1993, **30**, 841 (*synth, oxides*)

2-Amino-6-methylpyrazine, 8CI A-1-00181

6-Methylpyrazinamine, 9CI

[5521-56-2]

$C_5H_7N_3$ M 109.1
Cryst. (C_6H_6 or cyclohexane). Mp 128-129° (121-122°).

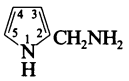
N-*Ac:* [5594-16-1].
$C_7H_9N_3O$ M 151.1 Cryst. (H_2O or MeOH). Mp 170°.

Weijlard, J. *et al, J.A.C.S.*, 1945, **67**, 802 (*synth*)
Sharefkin, D.M., *J.O.C.*, 1959, **24**, 345 (*synth, N-Ac*)
Pitré, D. *et al, Chem. Ber.*, 1966, **99**, 364 (*synth, N-Ac*)
Sato, N., *J. Het. Chem.*, 1980, **17**, 142 (*synth*)

2-(Aminomethyl)pyrrole A-1-00182

1H-Pyrrole-2-methanamine, 9CI

[64608-72-6]



$C_5H_8N_2$ M 96.1
Yellow liq. Bp_8 96°. n_D^{18} 1.5533.

N-*Me:* [26052-05-1]. *2-(Methylaminomethyl) pyrrole*
$C_6H_{10}N_2$ M 110.1 Liq. Bp_{11} 84-85°.

N,N-*Di-Me:* [14745-84-7]. *2-(Dimethylaminomethyl)pyrrole*
$C_7H_{12}N_2$ M 124.1 Cryst. (hexane). Mp 64°. Bp_{19} 94°.

1-Ph: [154123-03-2]. *1-Phenyl-1H-pyrrole-2-methanamine, 9CI*
$C_{11}H_{12}N_2$ M 172.2 Oil.

Putochin, N., *Ber.*, 1926, **59**, 1987 (*synth*)
Herz, W. *et al, J.A.C.S.*, 1947, **69**, 1698 (*N-Me, NN-di-Me*)
Flament, I. *et al, Helv. Chim. Acta*, 1977, **60**, 1872 (*synth*)
Korakas, D. *et al, Synthesis*, 1994, 164 (*1-Ph*)
Katritzky, A.R. *et al, Synth. Commun.*, 1995, **25**, 2631 (*1-Ph*)

3-(Aminomethyl)pyrrole A-1-00183

1H-Pyrrole-3-methanamine

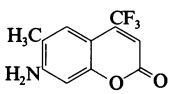
$C_5H_8N_2$ M 96.1

1-Me: [20863-72-3].
$C_6H_{10}N_2$ M 110.1 Liq. Bp_{20} 95-97°.

Paul, R. *et al, Bull. Soc. Chim. Fr.*, 1968, 2134.

7-Amino-6-methyl-4-(trifluoromethyl)-2*H*-1-benzopyran-2-one, 9CI A-1-00184

7-Amino-6-methyl-4-(trifluoromethyl)coumarin



$C_{11}H_8F_3NO_2$ M 243.1

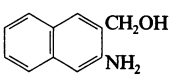
N-*Et:* [55804-70-1]. *7-Ethylamino-6-methyl-4-trifluoromethylcoumarin. Coumarin 503*
$C_{13}H_{12}F_3NO_2$ M 271.2 Laser dye. λ_{max} 503 nm.

Reynolds, G.A. *et al, Opt. Commun.*, 1975, **13**, 222 (*use, N-Et*)
Chinnakali, K. *et al, Acta Cryst. C*, 1992, **48**, 386 (*cryst struct, N-Et*)

3-Amino-2-naphthalenemethanol, 9CI A-1-00185

2-Amino-3-hydroxymethylnaphthalene

[141281-58-5]



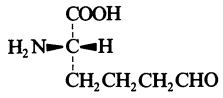
$C_{11}H_{11}NO$ M 173.2
Powder. Mp 181-183°.

Taffarel, E. *et al, J.O.C.*, 1994, **59**, 823 (*synth, pmr, cmr*)

2-Amino-6-oxohexanoic acid A-1-00186

6-Oxonorleucine, 9CI. 5-Formylnorvaline, 8CI. α-Aminoadipic semialdehyde. 2-Aminoadipaldehydic acid. Allysine

[1962-83-0]



(*S*)-*form*

$C_6H_{11}NO_3$ M 145.1

In equil. with the anhydro-form 2,3,4,5-Tetrahydro-2-pyridinecarboxylic acid, T-0-01579. Does not show typical aldehyde reactions.

(*S*)-*form*

L-form

Found in collagen, elastin and heart muscle. Intermed. in metab. and biosynth. of lysine. $[\alpha]_D^{25}$ −5.1 (c, 3 in H_2O) (ca. 90% pure).

(±)-*form*

Obt. only in soln.

2,4-Dinitrophenylhydrazone: Cryst. (EtOH). Mp 116-117°. Formed only slowly (5 days at 5°).

N-*Ac:*

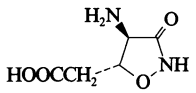
$C_8H_{13}NO_4$ M 187.1 Mp 95-96°.

Aspen, A.J. *et al, Biochemistry*, 1962, **1**, 600.

Basso, L.V. *et al, J. Biol. Chem.*, 1962, **237**, 2239.

Rodwell, V.W., *Methods Enzymol., Part B*, 1971, **17**, 188 (*synth, bibl*)

4-Amino-3-oxo-5-isoxazolidineacetic acid, 9CI, 8CI A-1-00187



(3*RS*,4*RS*)-*form*

$C_5H_8N_2O_4$ M 160.1

(3*RS*,4*RS*)-*form* [23172-64-7]

(±)-trans-*form*

No phys. props. reported.

(3*RS*,4*SR*)-*form* [23172-63-6]

(±)-cis-*form*

Cryst. (EtOH aq.). Mp 163° dec.

[2644-50-0, 2644-51-1]

Khomutov, R.M. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1965, **161**, 1227 (*synth, cis, trans*)

Kamiya, T., *Chem. Pharm. Bull.*, 1969, **17**, 895 (*synth, cis*)

(2-Aminooxyethyl)phosphonic acid A-1-00188

[105406-29-9]

$H_2NOCH_2CH_2P(O)(OH)_2$

$C_2H_8NO_4P$ M 141.0

Cryst. (EtOH aq.). Mp 202°.

Mono-Me ester: Mono-methyl (2-aminooxyethyl)phosphonate

$C_3H_{10}NO_4P$ M 155.0 Solid. Mp 179-181° dec.

Di-Et ester: Diethyl (2-aminooxyethyl) phosphonate

$C_6H_{16}NO_4P$ M 197.1 Oil (as hydrochloride).

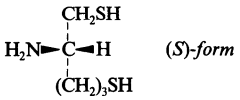
[105406-27-7]

Khomutov, A.R. *et al, Bioorg. Khim.*, 1986, **12**, 1662; *Sov. J. Bioorg. Chem. (Engl. Transl.)*, 1986, **12**, 887 (*synth, pmr*)

Khomutov, A.R. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1986, 1202; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1986, 1092.

2-Amino-1,5-pentanedithiol, 9CI A-1-00189

2-Amino-1,5-dimercaptopentane



(*S*)-*form*

$C_5H_{13}NS_2$ M 151.2

(*S*)-*form*

Hydrochloride: [23356-91-4].

Oil.

Cyclic disulfide: [23356-90-3]. *1,2-Dithiepan-4-amine, 8CI. 4-Amino-1,2-dithiepane*

Cryst. (EtOH) (as hydrochloride). Mp 229.5-230°. $[\alpha]_D^{26}$ −35 (c, 0.74 in H_2O).

Herbrandson, H.F. *et al, J. Med. Chem.*, 1969, **12**, 620 (*synth*)

Chauoel, E.N. *et al, J. Med. Chem.*, 1994, **37**, 2950 (*synth, pmr*)

3-Amino-1,5-pentanedithiol A-1-00190

3-Amino-1,5-dimercaptopentane

$HSH_2CCH_2CH(NH_2)CH_2CH_2SH$

$C_5H_{13}NS_2$ M 151.2

Hydrochloride: [21925-82-6].

Cryst. solid (2-propanol). Mp 128-132°.

Cyclic disulfide: [21925-83-7]. *1,2-Dithiepan-5-amine, 8CI. 5-Amino-1,2-dithiepane*

$C_5H_{11}NS_2$ M 149.2 Cryst. (EtOH) (as hydrochloride). Mp 224-228°.

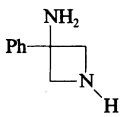
[21925-78-0]

Herbrandson, H.F. *et al, J. Med. Chem.*, 1969, **12**, 617 (*synth, ir*)

3-Amino-3-phenylazetidine A-1-00191

3-Phenyl-3-azetidinamine, 9CI

[161838-95-5]



$C_9H_{12}N_2$ M 148.2

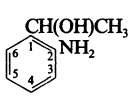
Powder (as hydrochloride). Mp 120° (hydrochloride). CAS no. refers to hydrochloride.

Bacqué, E. *et al, Synth. Commun.*, 1995, **25**, 803 (*synth, ir, pmr*)

1-(2-Aminophenyl)ethanol A-1-00192

2-Amino-α-methylbenzenemethanol, 9CI. (2-Aminophenyl)methylcarbinol

[10517-50-7]



$C_8H_{11}NO$ M 137.1

(+)-*form*

Needles (C_6H_6/hexane). Mp 49-54°. $[\alpha]_D^{18}$ +4.5 (c, 16.2 in MeOH).

(−)-*form*

Needles (C_6H_6/hexane). Mp 54-59°. $[\alpha]_D^{16}$ −4.1 (c, 13.6 in MeOH).

(±)-*form* [57793-77-8]

Needles (petrol). Mp 48-50°.

Nagai, U. *et al, Tetrahedron*, 1965, **21**, 1701 (*synth, ir*)

Fleming, I. *et al, J.C.S. Perkin 1*, 1986, 349 (*synth, pmr*)

1-(3-Aminophenyl)ethanol A-1-00193

3-Amino-α-methylbenzenemethanol, 9CI. (3-Aminophenyl)methylcarbinol

[2454-37-7]

$C_8H_{11}NO$ M 137.1

(±)-*form* [138561-59-8]

Cryst. (toluene or CCl_4); plates (C_6H_6). Mp 68-69°.

N-*Me:*

$C_9H_{13}NO$ M 151.2 Liq. Bp_2 140-142°.

N-*Et:*

$C_{10}H_{15}NO$ M 165.2 Liq. Bp_2 135-138°.

Marvel, C.S. *et al, J.A.C.S.*, 1946, **68**, 185 (*synth, N-Me, N-Et*)

Leonard, N.J. *et al, J.O.C.*, 1946, **11**, 405 (*synth*)

Ferrutti, P., *Chim. Ind. (Milan)*, 1965, **47**, 496 (*synth*)

Jones, A.G., *J. Chem. Educ.*, 1989, **66**, 611 (*synth, ir*)

1-(4-Aminophenyl)ethanol A-1-00194

4-Amino-α-methylbenzenemethanol, 9CI. (4-Aminophenyl)methylcarbinol

$C_8H_{11}NO$ M 137.1

(±)-*form* [93453-80-6]

Cryst.(H_2O). Mp 92-93°.

N,N-*Di-Me:* [5338-94-3].

$C_{10}H_{15}NO$ M 165.2 Yellow prisms (petrol). Mp 61°.

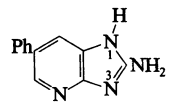
Sachs, F. *et al, Ber.*, 1905, **38**, 511 (*NN-di-Me*)

Allen, M.J. *et al, J.A.C.S.*, 1950, **72**, 115 (*synth*)

Clerici, A. *et al, J.O.C.*, 1985, **50**, 76 (*pmr*)

Knauer, B. *et al, Annalen*, 1995, 677 (*NN-di-Me*)

2-Amino-6-phenylimidazo[4,5-*b*]pyridine A-1-00195



1*H*-*form*

$C_{12}H_{10}N_4$ M 210.2

***1H*-form**

1-Me: [105650-23-5]. *1-Methyl-6-phenyl-1H-imidazo[4,5-b]pyridin-2-amine, 9CI. 2-Amino-1-methyl-6-phenyl-1H-imidazo[4,5-b] pyridine. PhIP*

$C_{13}H_{12}N_4$ M 224.2 Mutagen isol. from grilled meat and fish. Solid. Mp 327-328°.

▶ Mutagen.

***3H*-form**

3-Me: 2-Amino-3-methyl-6-phenyl-3H-imidazo[4,5-b]pyridine

$C_{13}H_{12}N_4$ M 224.2 Mp 217°.

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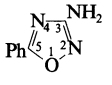
▶ Mutagen.

Knize, M.G. *et al*, *Heterocycles*, 1986, **24**, 1815 (*synth, ir, uv, pmr, cmr*)
Lindström, S. *et al*, *Acta Chem. Scand.*, 1993, **47**, 805 (*bibl*)

3-Amino-5-phenyl-1,2,4-oxadiazole A-1-00196

5-Phenyl-1,2,4-oxadiazol-3-amine, 9CI

[7788-14-9]



$C_8H_7N_3O$ M 161.1
Needles (H_2O). Mp 168-169°.

N-*Me:* [115822-11-2].
$C_9H_9N_3O$ M 175.1 Mp 123°.

Wieland, H. *et al*, *Ber.*, 1907, **40**, 1680 (*synth*)
Adams, P. *et al*, *J.O.C.*, 1953, **18**, 934 (*synth*)
Strani, G. *et al*, *Gazz. Chim. Ital.*, 1963, **93**, 482 (*synth*)
Huffman, K.R. *et al*, *J.O.C.*, 1963, **28**, 1812 (*synth*)
Eloy, F. *et al*, *Bull. Soc. Chim. Belg.*, 1964, **73**, 518 (*synth*)
Warburton, W.K., *J.C.S.(C)*, 1966, 1522 (*synth, uv, ir, pmr*)
Kraft, R. *et al*, *Org. Mass Spectrom.*, 1976, **11**, 304 (*ms*)

5-Amino-3-phenyl-1,2,4-oxadiazole A-1-00197

3-Phenyl-1,2,4-oxadiazol-5-amine, 9CI

[3663-37-4]

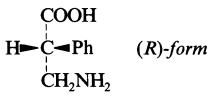
$C_8H_7N_3O$ M 161.1
Cryst. (H_2O or C_6H_6). Mp 154-155° (147-148°).

Palazzo, G. *et al*, *Gazz. Chim. Ital.*, 1960, **90**, 1290 (*synth*)
Huffman, K.R. *et al*, *J.O.C.*, 1963, **28**, 1816 (*synth*)
Eloy, F. *et al*, *Helv. Chim. Acta*, 1966, **49**, 1430 (*synth*)
Warburton, W.K., *J.C.S.(C)*, 1966, 1522 (*synth, uv, ir, pmr*)
Kraft, R. *et al*, *Org. Mass Spectrom.*, 1976, **11**, 304 (*ms*)

3-Amino-2-phenylpropanoic acid A-1-00198

Updated Entry replacing A-0-03480
α-(*Aminomethyl*)*benzeneacetic acid, 9CI. β-Aminohydratropic acid, 8CI*

[4370-95-0]



(R)-form

$C_9H_{11}NO_2$ M 165.1
Abs. config. revised in 1995.

(R)-form [1076-51-3]
Cryst. (EtOH). Mp 224-225°. $[\alpha]_D^{21}$ +95 (c, 0.2 in H_2O).

(±)-***form*** [54422-64-9]
Spar. sol. H_2O, org. solvs. Mp 233°.

Me ester: [99075-25-9].
$C_{10}H_{13}NO_2$ M 179.2 Cryst. solid (as hydrochloride).

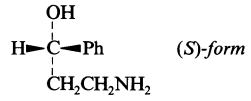
[1076-51-3]

Mckenzie, A. *et al*, *J.C.S.*, 1925, **127**, 85 (*synth*)
Garbarino, J.A. *et al*, *J.C.S. Perkin 1*, 1981, 906 (*resoln*)
Cox, R.J. *et al*, *J.C.S. Perkin 1*, 1991, 2537 (*synth, pmr, cmr, ir*)
D'Souza, A.A. *et al*, *J.C.S. Perkin 1*, 1995, 1 (*cryst struct, abs config*)

3-Amino-1-phenyl-1-propanol A-1-00199

α-(*2-Aminoethyl*)*benzenemethanol, 9CI. α-(2-Aminoethyl)benzyl alcohol, 8CI. γ-Hydroxy-γ-phenylpropylamine*

[5053-63-4]



(S)-form

$C_9H_{13}NO$ M 151.2

(S)-form [130194-42-2]
Cryst. (toluene). Mp 56°. $[\alpha]_D^{25}$ −43.6 (c, 1 in MeOH).

N-*Me:* [114133-37-8].
$C_{10}H_{15}NO$ M 165.2 Oil. $[\alpha]_D^{25}$ −38.2 (c, 1.0 in $CHCl_3$).

(±)-***form*** [59198-39-9]
Cryst. (C_6H_6). Mp 63.5-64.5°.

N-*Benzoyl:* [80213-06-5].
$C_{16}H_{17}NO_2$ M 255.3 Cryst. (EtOH aq.). Mp 85-86°.

N-*Me:* [153745-64-3].
Oil. Bp_2 109°.

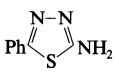
[42142-52-9]

Davies, R.E. *et al*, *J.A.C.S.*, 1945, **67**, 1466 (*synth, N-benzoyl*)
English, J. *et al*, *J.A.C.S.*, 1956, **78**, 4057 (*synth*)
Meisel, S.L. *et al*, *J.A.C.S.*, 1956, **78**, 4782 (*synth*)
Iwai, I. *et al*, *Chem. Pharm. Bull.*, 1963, **11**, 1049 (*N-Me*)
Shih, Y.-E. *et al*, *Heterocycles*, 1986, **24**, 1599 (*synth*)
Kumar, A. *et al*, *Indian J. Chem., Sect. B*, 1992, **31**, 803 (*N-Me*)
Chênevert, R. *et al*, *Tetrahedron*, 1992, **48**, 6769 (*N-Me*)
Mitchell, D. *et al*, *Synth. Commun.*, 1995, **25**, 1231 (*S-form, synth, ir, pmr, cmr, ms*)

2-Amino-5-phenyl-1,3,4-thiadiazole, 8CI A-1-00200

5-Phenyl-1,3,4-thiadiazol-2-amine, 9CI

[2002-03-1]



$C_8H_7N_3S$ M 177.2
Plates (EtOH aq.). Mp 224° (211-213°).

N-*Ph:* [1437-57-6]. N,*5-Diphenyl-1,3,4-thiadiazol-2-amine, 9CI*
$C_{14}H_{11}N_3S$ M 253.3 Cryst. (EtOH). Mp 200°.

Hoggarth, E., *J.C.S.*, 1949, 1163 (*synth*)
Testa, E. *et al*, *Gazz. Chim. Ital.*, 1958, **88**, 812 (*ir, uv*)
Svanholm, U., *Acta Chem. Scand.*, 1972, **26**, 459 (*pmr*)
Kirkien-Rzeszotarski, A.M. *et al*, *J. Het. Chem.*, 1977, **14**, 401 (*ms*)
Sharma, S. *et al*, *Indian J. Chem., Sect. B*, 1985, **24**, 1154 (*synth*)
Isoda, S. *et al*, *Chem. Pharm. Bull.*, 1992, **40**, 357 (*synth*)
Mourad, A.-F.E. *et al*, *Annalen*, 1994, 989 (*synth, pmr, ir, ms*)

3-Amino-2-propenoic acid A-1-00201

$H_2NCH{=}CHCOOH$

$C_3H_5NO_2$ M 87.0

(Z)-form

Nitrile: [24532-82-9]. *1-Amino-2-cyanoethylene*
$C_3H_4N_2$ M 68.0 Low melting solid. Mp 7-8°. $Bp_{0.02}$ 65°.

[19866-98-9]

Sieveking, H.U. *et al*, *Angew. Chem., Int. Ed.*, 1969, **8**, 458 (*synth, pmr, ir, nitrile*)
Xiang, Y. *et al*, *Helv. Chim. Acta*, 1994, **77**, 2209 (*nitrile, synth, uv, ir, pmr, cmr*)

(3-Aminopropyl) phenylphosphinic acid A-1-00202

[123691-73-6]

$PhP(O)(OH)CH_2CH_2CH_2NH_2$

$C_9H_{14}NO_2P$ M 199.1

Et ester: [123691-72-5]. *Ethyl (3-aminopropyl) phenylphosphinate*
$C_{11}H_{18}NO_2P$ M 227.2 Liq. $Bp_{0.5}$ 110°.

Lu, X. *et al*, *Heteroat. Chem.*, 1992, **3**, 551 (*Et ester, synth, ir, ms, pmr*)

(3-Aminopropyl)phosphinic acid, 9CI A-1-00203

[103680-47-3]

$H_2NCH_2CH_2CH_2PH(O)OH$

$C_3H_{10}NO_2P$ M 123.0
Muscle relaxant, anticonvulsant, analgesic. Powder. Mp 209-213°.

Dingwall, J.G. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1987, **30**, 571 (*rev*)
Dingwall, J.G. *et al*, *Tetrahedron*, 1989, **45**, 3787 (*synth, pmr, P-31 nmr*)

6-Amino-3-pyridazinecarboxylic acid, 9CI A-1-00204

[59772-58-6]

$C_5H_5N_3O_2$ M 139.1
Cryst. Mp 168-170°.

Hydrochloride: Cryst. Mp 243-245°.

Me ester: [98140-96-6].
$C_6H_7N_3O_2$ M 153.1 Cryst. Mp 200-201°.

Et ester:
$C_7H_9N_3O_2$ M 167.1 Cryst. Mp 168-169°.

Amide: [98021-37-5].
$C_5H_6N_4O$ M 138.1 Mp 264°.

Mitsui, S. *et al*, *Nippon Kagaku Zasshi*, 1957, **78**, 577; *CA*, **53**, 5275f.
Mourad, A.E. *et al*, *J. Het. Chem.*, 1992, **29**, 1583 (*synth, ir, pmr*)

6-Amino-2-pyridinecarboxylic acid, 9CI A-1-00205

6-Aminopicolinic acid, 8CI

[23628-31-1]

$C_6H_6N_2O_2$ M 138.1
Cryst. (H_2O). Mp 316-318°.

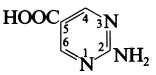
Me ester:
$C_7H_8N_2O_2$ M 152.1 Solid. Mp 88°.

Et ester:
$C_8H_{10}N_2O_2$ M 166.1 Solid. Mp 56°.
Amide:
$C_6H_7N_3O$ M 137.1 Cryst. (H_2O). Mp 145°.
N-*Ac:* [26893-72-1].
$C_8H_8N_2O_3$ M 180.1 Cryst. Mp 220°.
N-*Ac, Me ester:*
$C_9H_{10}N_2O_3$ M 194.1 Cryst. (H_2O). Mp 180°.
N-*Ac, amide:*
$C_8H_9N_3O_2$ M 179.1 Cryst. (EtOH). Mp 223°.

Ferrari, G. *et al, Farmaco, Ed. Sci.*, 1959, **14**, 594; *CA*, **54**, 6709b (*synth, derivs*)
Moser, R.J. *et al, Org. Mass Spectrom.*, 1970, **4**, 555 (*ms*)
Brown, E.V. *et al, J.O.C.*, 1971, **36**, 454 (*synth, N-Ac*)
Janecka, A. *et al, J. Med. Chem.*, 1994, **37**, 2238 (*synth, pmr*)

2-Amino-5-pyrimidinecarboxylic acid A-1-00206

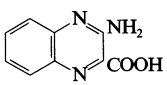
[3167-50-8]



$C_5H_5N_3O_2$ M 139.1
Needles (H_2O). Mp >300°.
Et ester:
$C_7H_9N_3O_2$ M 167.1 Needles (H_2O). Mp 147-149°.
Nitrile: 2-Amino-5-cyanopyrimidine
$C_5H_4N_4$ M 120.1 Prisms (EtOH). Mp *ca.* 260° dec.

Ballard, E. *et al, J.A.C.S.*, 1942, **64**, 794 (*synth, Et ester*)
English, J.P. *et al, J.A.C.S.*, 1946, **68**, 1039 (*nitrile, synth*)
Takamizawa, A. *et al, Chem. Pharm. Bull.*, 1964, **12**, 804 (*synth, Et ester*)
Takamizawa, A. *et al, J.O.C.*, 1964, **29**, 1740 (*nitrile, synth, uv, ir*)
Schenone, P. *et al, J. Het. Chem.*, 1990, **27**, 295 (*synth, uv, ir, pmr*)

3-Amino-2-quinoxalinecarboxylic acid A-1-00207

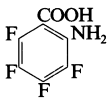


$C_9H_7N_3O_2$ M 189.1
Amide: [67568-30-3].
$C_9H_8N_4O$ M 188.1 Cryst. (MeOH). Mp 265°.
Hydrazide: [61857-84-9].
$C_9H_9N_5O$ M 203.2 Yellow solid. Mp 201°.
Nitrile: [36597-16-7]. *2-Amino-3-cyanoquinoxaline*
$C_9H_6N_4$ M 170.1 Bright yellow solid (EtOAc). Mp 201°.
Nitrile, 4-oxide:
$C_9H_6N_4O$ M 186.1 Orange solid. Mp 266°.
Nitrile, 1,4-dioxide: [23190-84-3].
$C_9H_6N_4O_2$ M 202.1 Cryst. (dioxan). Mp 190° (230° dec.).

Borah, H.N. *et al, Heterocycles*, 1984, **22**, 2323.
Monge, A. *et al, J. Med. Chem.*, 1993, **36**, 2745.
Monge, A. *et al, J. Het. Chem.*, 1994, **31**, 1135 (*derivs*)

2-Amino-3,4,5,6-tetrafluorobenzoic acid, 9CI A-1-00208

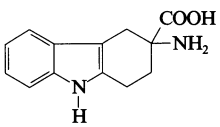
Tetrafluoroanthranilic acid, 8CI
[1765-42-0]



$C_7H_3F_4NO_2$ M 209.1
Cryst. (H_2O). Mp 141-142°.
Et ester: [34941-14-5].
$C_9H_7F_4NO_2$ M 237.1 Cryst. (petrol). Mp 65-66°.
Amide:
$C_7H_4F_4N_2O$ M 208.1 Cryst. (H_2O). Mp 140-141°.
Nitrile: 2-Cyano-3,4,5,6-tetrafluoroaniline
$C_7H_2F_4N_2$ M 190.1 Cryst. (C_6H_6). Mp 89-90°. Bp_{14} 115°.

Gething, B. *et al, J.C.S.*, 1961, 1574 (*synth, ir*)
Belf, L.J. *et al, Tetrahedron*, 1967, **23**, 4719.
Brooke, G.M. *et al, Tetrahedron*, 1971, **27**, 5653.

3-Amino-1,2,3,4-tetrahydro-3-carbazolecarboxylic acid A-1-00209

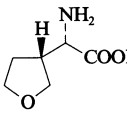


$C_{13}H_{14}N_2O_2$ M 230.2
(±)-***form***
Mp 300-302° dec.
N-*Ac:*
$C_{15}H_{16}N_2O_3$ M 272.3 Cryst. Mp 278-281° dec.

Britten, A. *et al, J.C.S. Perkin 1*, 1974, 1824 (*synth*)
Yu, H.T. *et al, J.A.C.S.*, 1995, **117**, 34 (*synth, cryst struct*)

α-Aminotetrahydro-3-furanacetic acid, 9CI A-1-00210

2-Amino-2-(tetrahydrofuran-3-yl)acetic acid. Tetrahydro-3-furanylglycine

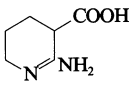


(*2S,3'R*)-*form*

$C_6H_{11}NO_3$ M 145.1
(***2S,3'R*)-*form*** [150331-97-8]
Solid. $[\alpha]_D^{23}$ −17.7 (c, 1.29 in H_2O).
(***2S,3'S*)-*form*** [150331-99-0]
Solid. $[\alpha]_D^{23}$ +10.3 (c, 1.125 in H_2O).

Ghosh, A.K. *et al, J. Med. Chem.*, 1993, **36**, 2300 (*synth, pmr*)

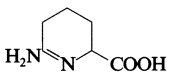
2-Amino-3,4,5,6-tetrahydro-3-pyridinecarboxylic acid, 9CI A-1-00211



$C_6H_{10}N_2O_2$ M 142.1
(±)-***form*** [158832-69-0]
Oil (as hydrochloride).
Me ester: [158832-56-5].
$C_7H_{12}N_2O_2$ M 156.1 Cryst. ($MeOH/Et_2O$) (as hydrochloride). Mp 138-139°.
[158832-43-0]

Dunbar, P.G. *et al, J. Med. Chem.*, 1994, **37**, 2774 (*synth, ir, pmr*)

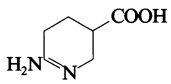
6-Amino-2,3,4,5-tetrahydro-2-pyridinecarboxylic acid A-1-00212



$C_6H_{10}N_2O_2$ M 142.1
(±)-***form*** [158832-72-5]
Cryst. (as hydrochloride).
Me ester: [158832-62-3].
$C_7H_{12}N_2O_2$ M 156.1 Cryst. (EtOH) (as hydrochloride). Mp 132-134°.
[158832-49-6]

Dunbar, P.G. *et al, J. Med. Chem.*, 1994, **37**, 2774 (*synth, pmr, ir*)

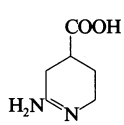
6-Amino-2,3,4,5-tetrahydro-3-pyridinecarboxylic acid A-1-00213



$C_6H_{10}N_2O_2$ M 142.1
(±)-***form*** [158832-71-4]
Cryst. ($EtOH/Et_2O$) (as hydrochloride). Mp 261-263° (hydrochloride).
Me ester: [158832-58-7].
$C_7H_{12}N_2O_2$ M 156.1 Cryst. ($MeOH/Et_2O$) (as hydrochloride). Mp 181-183°.
Et ester:
$C_8H_{14}N_2O_2$ M 170.2 Cryst. ($EtOH/Et_2O$) (as hydrochloride). Mp 175-177°.
[158832-45-2, 158930-48-4]

Dunbar, P.G. *et al, J. Med. Chem.*, 1994, **37**, 2774 (*synth, ir, pmr*)

6-Amino-2,3,4,5-tetrahydro-4-pyridinecarboxylic acid, 9CI A-1-00214



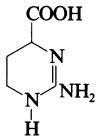
$C_6H_{10}N_2O_2$ M 142.1
(±)-***form*** [158832-70-3]
Cryst. (as hydrochloride).
Me ester: [158832-57-6].

$C_7H_{12}N_2O_2$ M 156.1 Cryst. (MeOH/Et_2O) (as hydrochloride). Mp 180-181°.

[158832-44-1]

Dunbar, P.G. *et al, J. Med. Chem.*, 1994, **37**, 2774 (*synth, ir, pmr*)

2-Amino-1,4,5,6-tetrahydro-4-pyrimidinecarboxylic acid A-1-00215



$C_5H_9N_3O_2$ M 143.1

(±)-*form* [158930-47-3]
Cryst. (MeOH/Et_2O). Mp 199-200°.

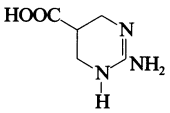
Me ester: [158832-63-4].
$C_6H_{11}N_3O_2$ M 157.1 Needles (MeOH/THF) (as hydrochloride). Mp 106-108°.

[158832-50-9]

Dunbar, P.G. *et al, J. Med. Chem.*, 1994, **37**, 2774 (*synth, ir, pmr*)

2-Amino-1,4,5,6-tetrahydro-5-pyrimidinecarboxylic acid A-1-00216

[158832-73-6]



$C_5H_9N_3O_2$ M 143.1

(±)-*form*
Cryst. (EtOH/Et_2O) (as hydrochloride). Mp 190-192° (hydrochloride).

Me ester: [158832-64-5].
$C_6H_{11}N_3O_2$ M 157.1 Cryst. (MeOH/Et_2O) (as hydrochloride). Mp 167-168° (hydrochloride).

Et ester:
$C_7H_{13}N_3O_2$ M 171.1 Cryst. (EtOH/Et_2O) (as hydrochloride). Mp 154-155° (hydrochloride).

Isopropyl ester:
$C_8H_{15}N_3O_2$ M 185.2 Pale yellow cryst. (2-propanol/Et_2O) (as hydrochloride). Mp 145-146° (hydrochloride).

[158832-51-0]

Dunbar, P.G. *et al, J. Med. Chem.*, 1994, **37**, 2774 (*synth, ir, pmr*)

2-Amino-3-thiophenecarboxaldehyde, 9CI A-1-00217

2-Amino-3-formylthiophene

[40341-23-9]

C_5H_5NOS M 127.1

Capperucci, A. *et al, J.O.C.*, 1995, **60**, 2254 (*synth, ir, pmr, cmr, ms*)

3-Amino-2-thiophenecarboxaldehyde, 9CI A-1-00218

3-Amino-2-formylthiophene

[56489-01-1]

C_5H_5NOS M 127.1
Cryst. (EtOH aq.). Mp 68.0-70.0°.

Gronowitz, S. *et al, Acta Chem. Scand., Ser. B*, 1975, **29**, 224 (*synth, ir, pmr*)
Ah-Kow, G. *et al, Bull. Soc. Chim. Fr.*, 1976, 151 (*synth, pmr*)

5-Amino-2-thiophenecarboxaldehyde, 9CI A-1-00219

2-Amino-5-formylthiophene

[57500-50-2]

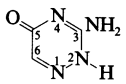
C_5H_5NOS M 127.1

Capperucci, A. *et al, J.O.C.*, 1995, **60**, 2254 (*synth, ir, pmr, cmr, ms*)

3-Amino-1,2,4-triazin-5(2*H*)-one, 9CI A-1-00220

3-Amino-5-hydroxy-1,2,4-triazine. 3-Amino-1,2,4-triazin-5-ol. 6-Azaisocytosine

[1121-90-0]



$C_3H_4N_4O$ M 112.0
Exhibits weak inhibitory activity on nucleic acid synthesis. Needles. Mp >300°.

3N-Me:
$C_4H_6N_4O$ M 126.1 Cryst. (H_2O). Mp 321°.

3N,3N-Di-Me:
$C_5H_8N_4O$ M 140.1 Cryst. (EtOH). Mp 280-283°.

3N-Ph:
$C_9H_8N_4O$ M 188.1 Cryst. (DMF). Mp 280-283°.

2-β-D-Arabinofuranosyl: [19131-40-9].
$C_8H_{12}N_4O_5$ M 244.2 Solid.

2-β-D-Ribofuranosyl: [15147-69-0]. *6-Azaisocytidine*
$C_8H_{12}N_4O_5$ M 244.2 Cryst. Mp 260-261° dec. $[\alpha]_D^{25}$ +81.6 (c, 0.46 in DMSO).

Gut, J. *et al, Coll. Czech. Chem. Comm.*, 1966, **31**, 2014 (*synth, deriv*)
Zemlicka, J. *et al, Coll. Czech. Chem. Comm.*, 1967, **32**, 576 (*ribosyl deriv*)
Delia, T.J. *et al, J. Carbohydr., Nucleosides, Nucleotides*, 1977, **4**, 349 (*arabinosyl*)
Lovelette, C.A. *et al, J. Het. Chem.*, 1979, **16**, 585 (*synth, uv*)
Beranek, J. *et al, Coll. Czech. Chem. Comm.*, 1983, **48**, 2088; 1984, **49**, 2551 (*pharmacol*)
Jovanoic, M.V., *Heterocycles*, 1986, **24**, 951 (*synth, C-13 nmr, N-14 nmr*)

4-Amino-2-(trifluoromethyl) pyridine A-1-00221

2-(Trifluoromethyl)-4-pyridinamine, 9CI

[147149-98-2]

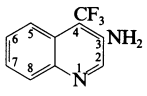
$C_6H_5F_3N_2$ M 162.1
Light orange solid. Mp 56-58°.

Webber, S.E. *et al, J. Med. Chem.*, 1993, **36**, 733 (*synth, ir, pmr*)

3-Amino-4-(trifluoromethyl) quinoline A-1-00222

4-(Trifluoromethyl)-3-quinolinamine

[155793-46-7]



$C_{10}H_7F_3N_2$ M 212.1
Mp 121-122°.

Kiselyov, A.S. *et al, Heterocycles*, 1994, **37**, 775.

5-Amino-8-(trifluoromethyl) quinoline A-1-00223

8-(Trifluoromethyl)-5-quinolinamine

$C_{10}H_7F_3N_2$ M 212.1
Mp 154-155°.

Strekowski, L. *et al, J. Het. Chem.*, 1994, **31**, 1413.

6-Amino-5-(trifluoromethyl) quinoline A-1-00224

5-(Trifluoromethyl)-6-quinolinamine

[155793-47-8]

$C_{10}H_7F_3N_2$ M 212.1
Mp 121-122°.

Kiselyov, A.S. *et al, Heterocycles*, 1994, **37**, 775.

8-Amino-5-(trifluoromethyl) quinoline A-1-00225

5-(Trifluoromethyl)-8-quinolinamine

$C_{10}H_7F_3N_2$ M 212.1
Mp 83-84°.

Strekowski, L. *et al, J. Het. Chem.*, 1994, **31**, 1413 (*synth, pmr, F-19 nmr*)

8-Amino-7-(trifluoromethyl) quinoline A-1-00226

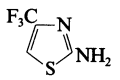
7-(Trifluoromethyl)-8-quinolinamine

$C_{10}H_7F_3N_2$ M 212.1
Oil.

Strekowski, L. *et al, J. Het. Chem.*, 1994, **31**, 1413 (*synth, pmr, F-19 nmr*)

2-Amino-4-(trifluoromethyl) thiazole A-1-00227

[349-49-5]



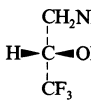
$C_4H_3F_3N_2S$ M 168.1
Cryst. (hexane). Mp 68-69.5° (66-68°). Bp_9 110-114°.

Dickey, J.B. *et al, J.O.C.*, 1955, **20**, 499 (*synth*)
Tanaka, K. *et al, J. Het. Chem.*, 1991, **28**, 907 (*synth, pmr*)

3-Amino-1,1,1-trifluoro-2-propanol, 9CI A-1-00228

2-Hydroxy-3,3,3-trifluoropropylamine

[431-38-9]



(*S*)-*form*

$C_3H_6F_3NO$ M 129.0

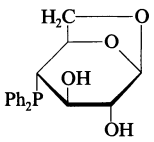
(S)-form [160706-71-8]
Solid. Mp 120-121°. $[\alpha]_D^{23}$ −19.54 (c, 1.3 in MeOH) (≥99% ee).

N,N-*Di-Et:* [160595-63-1].
$C_7H_{14}F_3NO$ M 185.1 Liq. Bp_{40} 100° (Kugelrohr). $[\alpha]_D^{22}$ −29.79 (c, 1.4 in MeOH) (96% ee).

(±)-form
Hydrochloride: Cryst. Mp 147-148°.

Jones, R.G., *J.A.C.S.*, 1948, **70**, 143 (*synth*)
Ramachandran, P.V. *et al*, *J.O.C.*, 1995, **60**, 41 (*synth, ir, pmr, cmr, F-19 nmr*)

1,6-Anhydro-4-deoxy-4-(diphenylphosphino) glucopyranose A-1-00229

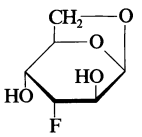


$C_{18}H_{19}O_4P$ M 330.3

β-D-form
2-(4-Methylbenzenesulfonyl), P-*oxide:* [136632-36-5].
$C_{25}H_{25}O_7PS$ M 500.5 Needles ($CHCl_3$ or $CHCl_3/Et_2O$). Mp 165-168°. $[\alpha]_D^{25}$ −41 (c, 0.1 in $CHCl_3$).

Li, C. *et al*, *Carbohydr. Res.*, 1991, **216**, 149 (*synth, uv, ir, ms*)

1,6-Anhydro-3-deoxy-3-fluoroaltropyranose A-1-00230



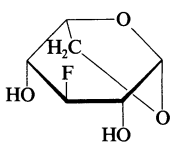
$C_6H_9FO_4$ M 164.1

D-form [38711-36-3]
Cryst. (Me_2CO/Et_2O). Mp 132-134°. $[\alpha]_D$ −194 (c, 0.18 in H_2O).

4-Benzyl: [23094-76-0].
$C_{13}H_{15}FO_4$ M 254.2 Cryst. Mp 102-103°. $[\alpha]_D$ −95 (c, 0.39 in $CHCl_3$).

Pacak, J. *et al*, *Chem. Comm.*, 1969, 77 (*deriv*)
Pacak, J. *et al*, *Coll. Czech. Chem. Comm.*, 1972, **37**, 2589 (*deriv, pmr, F-19 nmr*)

1,6-Anhydro-3-deoxy-3-fluoroidopyranose A-1-00231



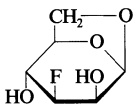
$C_6H_9FO_4$ M 164.1

L-form [39809-12-6]
Cryst. Mp 106-109°. $[\alpha]_D^{26}$ +106 (Me_2CO).

Di-Ac: [39809-13-7].
$C_{10}H_{13}FO_6$ M 248.2 Cryst. (Et_2O/petrol). Mp 83-84°. $[\alpha]_D$ +80.5 ($CHCl_3$).

Foster, A.B. *et al*, *Carbohydr. Res.*, 1972, **25**, 217 (*synth, pmr, F-19 nmr*)

1,6-Anhydro-3-deoxy-3-fluoromannopyranose A-1-00232



$C_6H_9FO_4$ M 164.1

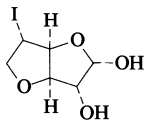
D-form [88142-85-2]
Cryst. (MeOH). Mp 158-160° (sinters at 110-134°). $[\alpha]_D$ −118 (c, 0.69 in H_2O).

Di-Ac: [88142-86-3].
$C_{10}H_{13}FO_6$ M 248.2 Syrup. $Bp_{0.15}$ 185° (bath). $[\alpha]_D$ −106 (c, 0.66 in $CHCl_3$).

Dibenzoyl: [88142-87-4].
$C_{20}H_{17}FO_6$ M 372.3 Cryst. ($EtOH/H_2O$). Mp 141-142°. $[\alpha]_D$ −186 (c, 0.5 in $CHCl_3$).

Cerny, M. *et al*, *Coll. Czech. Chem. Comm.*, 1983, **48**, 2693 (D-form, di-Ac, dibenzoyl)

3,6-Anhydro-5-deoxy-5-iodoidofuranose A-1-00233



$C_6H_9IO_4$ M 272.0

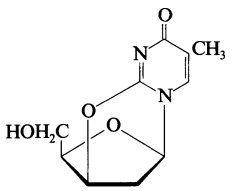
β-L-form
1,2-O-Isopropylidene: [35810-91-4].
$C_9H_{13}IO_4$ M 312.1 Cryst. Mp 67-68°. $[\alpha]_D^{20}$ +64.8 (c, 0.97 in $CHCl_3$).

Dax, K. *et al*, *Annalen*, 1981, 1768 (*isopropylidene, pmr*)

2,3′-Anhydrothymidine A-1-00234

*2,3-Dihydro-3-(hydroxymethyl)-8-methyl-2,5-methano-5*H,9H-*pyrimido[2,1-b][1,5,3] dioxazepin-9-one*, *9CI.* O^2*:3′-Cyclothymidine*

[15981-92-7]



$C_{10}H_{12}N_2O_4$ M 224.2
Intermed. in synth. of Zidovudine, A-0-04712. Needles (EtOH aq.). Mp 230°.

Michelson, A.M. *et al*, *J.C.S.*, 1955, 816 (*synth, uv*)
Rao, T.S. *et al*, *Chem. Comm.*, 1989, 997 (*synth, use*)

2,6-Anthracenedisulfonic acid A-1-00235

[61736-95-6]

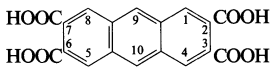
$C_{14}H_{10}O_6S_2$ M 338.3
Shiny plates (as K salt). Mp >400° (K salt).

[66601-74-9]

Schüler, G., *Ber.*, 1882, **15**, 1807 (*synth*)
Acquavella, M.F. *et al*, *J.O.C.*, 1994, **59**, 2894 (*synth, pmr*)

2,3,6,7-Anthracenetetracarboxylic acid, 9CI A-1-00236

[159113-89-0]



$C_{18}H_{10}O_8$ M 354.2
Pale yellow amorph. solid. Mp >300° dec.

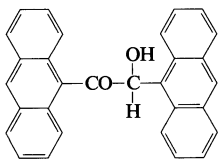
Tetra-Me ester: [113431-17-7].
$C_{22}H_{18}O_8$ M 410.3 Cryst. (MeCN). Mp 226-228°.

Morris, J.L. *et al*, *J.O.C.*, 1994, **59**, 6484 (*synth, ir, pmr, cmr, ester, cryst struct*)

9,9′-Anthroin A-1-00237

1,2-Di-9-anthracenyl-2-hydroxyethanone

[123230-60-4]



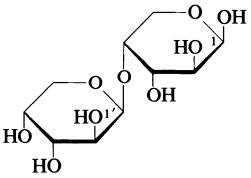
$C_{30}H_{20}O_2$ M 412.4

(±)-form
Dimorphic.

Ac:
$C_{32}H_{22}O_3$ M 454.5 Pale yellow cryst. (CH_2Cl_2/MeOH). Mp 238-240°.

Becker, H. *et al*, *Aust. J. Chem.*, 1991, **44**, 1737.

4-*O*-β-D-Arabinopyranosyl-D-arabinose A-1-00238



$C_{10}H_{18}O_9$ M 282.2

2,2′,3-Tri-Ac, 1-O-(3,7,11-trimethyl-2,6,10-dodecatrienyl): [143838-79-3].
$C_{31}H_{48}O_{12}$ M 612.7 Isol. from the coral *Sinularia* sp. Enhances glucose transport in rat adipocytes. Oil. $[\alpha]_D$ −196 (c, 0.7 in $CHCl_3$).

Shindo, T. *et al*, *Experientia*, 1992, **48**, 688 (*isol, pmr, cmr, ms*)

Avobenzone, INN, USAN A-1-00239

1-[4-(1,1-Dimethylethyl)phenyl]-3-(4-methoxyphenyl)-1,3-propanedione, *9CI. 1-*(p-tert-*Butylphenyl)-3-*(p-*methoxyphenyl)-1,3-propanedione. 4-(1,1-Dimethylethyl)-4′-methoxydibenzoylmethane. Parsol 1789. Parsol A. Clarins. Shade Uvagard*

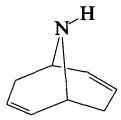
[70356-09-1]

$C_{20}H_{22}O_3$ M 310.3
Sunscreen agent. Cryst. (MeOH). Mp 83.5°. Component of Photoplex.

Ger. Pat., 2 945 125, (1980) (*Givaudan*); *CA*, **93**, 185967g (*synth*)
Kuhnert-Brandstaetter, M. *et al*, *Sci. Pharm.*, 1987, **55**, 27 (*polymorphism*)
Ikeda, K. *et al*, *J. Chromatogr.*, 1989, **482**, 240 (*hplc*)
Garmyn, M. *et al*, *J. Invest. Dermatol.*, 1989, **92**, 642 (*activity*)
Bissett, D.L. *et al*, *Photodermatology*, 1989, **6**, 228 (*activity*)
Martindale, *The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, London, 1993, 1234.

9-Azabicyclo[3.3.1]nona-2,6-diene, 9CI A-1-00240

[34668-51-4]

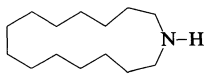


$C_8H_{11}N$ M 121.1
Hydrochloride: [34668-52-5]. Solid.
N-*Formyl:* [34668-91-2]. $C_9H_{11}NO$ M 149.1 Cryst. Mp 55-57°. Subl.$_{0.01}$ 55°.
N-*Benzenesulfonyl:* [34668-55-8]. Cryst. (CH_2Cl_2/hexane). Mp 162-164°.
N-*Me:* [34668-47-8]. $C_9H_{13}N$ M 135.2 Liq.
N-tert-*Butyl:* [54397-30-7]. $C_{12}H_{19}N$ M 177.2 Liq.
9-tert-*Butyl, hydrochloride:* [54397-31-8]. Solid (diisopropyl ether/EtOH 4:1).

Ganter, C. *et al*, *Helv. Chim. Acta*, 1971, **54**, 2069 (*synth*)
Cuthbertson, E. *et al*, *J.C.S. Perkin 1*, 1974, 1893 (*deriv, ms, ir, pmr*)

Azacyclopentadecane, 9CI, 8CI A-1-00241

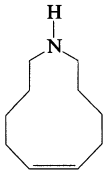
[295-49-8]



$C_{14}H_{29}N$ M 211.3
Mp 55°. pK_a 9.3.

Ruzicka, L. *et al*, *Helv. Chim. Acta*, 1949, **32**, 544 (*synth*)

Azacyclo-6-undecene, 9CI A-1-00242



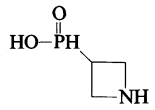
$C_{10}H_{19}N$ M 153.2
(*Z*)-*form* [126412-12-2] ***Keramaphidin C***
Isol. from the Okinawan marine sponge *Amphimedon* sp. Amorph. solid. Mp 106-109°.

Torisawa, Y. *et al*, *Tetrahedron*, 1991, **47**, 8067 (*synth*)
Tsuda, M. *et al*, *Tet. Lett.*, 1994, **35**, 4387 (*isol, ir, pmr, cmr*)

3-Azetidinephosphinic acid A-1-00243

3-Azetidinylphosphinic acid

[134150-82-6]

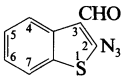


$C_3H_8NO_2P$ M 121.0
Cryst. Mp 189° dec.

Diel, P.J. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **56**, 1 (*synth, P-31 nmr*)

2-Azidobenzo[*b*]thiophene-3-carboxaldehyde A-1-00244

2-Azido-3-formylbenzo[b]*thiophene*



$C_9H_5N_3OS$ M 203.2
Cryst. Mp 91-94° dec. Unstable in light.

Chippendale, K.E. *et al*, *J.C.S. Perkin 1*, 1973, 129 (*synth*)
Degl'Innocenti, A. *et al*, *J.C.S. Perkin 1*, 1995, 2141 (*synth*)

3-Azidobenzo[*b*]thiophene-2-carboxaldehyde A-1-00245

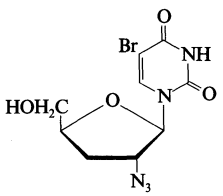
3-Azido-2-formylbenzo[b]*thiophene*

$C_9H_5N_3OS$ M 203.2
Cryst. Mp 88-90° dec.

Chippendale, K.E. *et al*, *J.C.S. Perkin 1*, 1973, 129 (*synth*)
Degl'Innocenti, A. *et al*, *J.C.S. Perkin 1*, 1995, 2141 (*synth*)

2′-Azido-5-bromo-2′,3′-dideoxyuridine A-1-00246

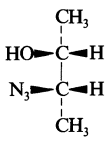
[126543-49-5]



$C_9H_{10}BrN_5O_4$ M 332.1
Solid. Mp 148-150°.

Warshaw, J.A. *et al*, *J. Med. Chem.*, 1990, **33**, 1663 (*synth, pmr, ir, uv*)

3-Azido-2-butanol A-1-00247



(2*R*,3*S*)-*form*

$C_4H_9N_3O$ M 115.1

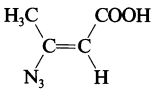
(2*R*,3*S*)-*form*
Liq. Bp_{20} 79-80°. $[\alpha]_D^{20}$ +43.1 (c, 2.5 in heptane).

(±)-*form*
Liq. Bp_{31} 83-84°. $n_D^{17.5}$ 1.4562. Presumably mixt. of diastereoisomers.

[110716-80-8]

Van der Werf, C.A. *et al*, *J.A.C.S.*, 1954, **76**, 1231 (*synth*)
Shustov, G.V. *et al*, *J.A.C.S.*, 1993, **115**, 10267 (*synth, pmr*)

3-Azido-2-butenoic acid A-1-00248



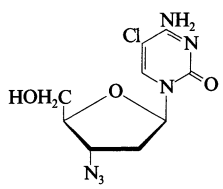
(*E*)-*form*

$C_4H_5N_3O_2$ M 127.1
(*E*)-*form*
cis-*form. 3-Aminoisocrotonic acid*
Me ester: [81777-19-7]. $C_5H_7N_3O_2$ M 141.1 Oil.
(*Z*)-*form*
trans-*form. 3-Aminocrotonic acid*
Me ester: [116270-29-2]. Yellowish plates. Mp 54-55° (51°). Subl.$_{0.1}$ 40°.

Priebe, H. *et al*, *Acta Chem. Scand., Ser. B*, 1987, **41**, 640 (*Me ester*)
Palacios, F. *et al*, *Org. Prep. Proced. Int.*, 1995, **27**, 171 (*Me ester*)

3′-Azido-5-chloro-2′,3′-dideoxycytidine, 9CI A-1-00249

[127492-31-3]

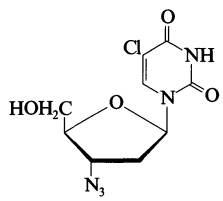


$C_9H_{11}ClN_6O_3$ M 286.6
Cryst. ($MeOH/Et_2O$). Mp 173-175° dec.

Van Aerschot, A. *et al*, *J. Med. Chem.*, 1990, **33**, 1833 (*synth, uv, ms, pmr, cmr*)

3′-Azido-5-chloro-2′,3′-dideoxyuridine, 9CI A-1-00250

[108441-51-6]



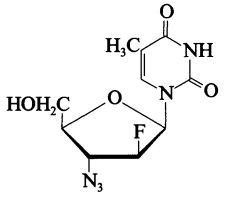
$C_9H_{10}ClN_5O_4$ M 287.6
Cryst. (EtOAc). Mp 170°.

Van Aerschot, A. *et al*, *J. Med. Chem.*, 1990, **33**, 1833 (*synth, uv, ir, ms, pmr, cmr*)

1-(3-Azido-2,3-dideoxy-2-fluoro-β-D-arabinofuranosyl) thymine A-1-00251

1-(3-Azido-2,3-dideoxy-2-fluoro-β-D-arabinofuranosyl)-5-methyl-2,4-(1H,3H)-pyrimidinedione, 9CI. F-AZT

[124424-26-6]



$C_{10}H_{12}FN_5O_4$ M 285.2

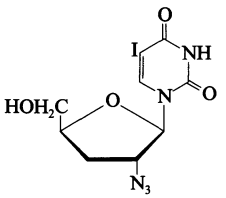
Does not show significant antiviral activity. Cryst. (Me_2CO/petrol). Mp 45-50°.

Watanabe, K.A. *et al, J. Med. Chem.*, 1990, **33**, 2145 (*synth, ir, pmr*)

Sterzycki, R.Z. *et al, J. Med. Chem.*, 1990, **33**, 2150 (*synth, pmr, cmr*)

2′-Azido-2′,3′-dideoxy-5-iodouridine A-1-00252

[126543-50-8]



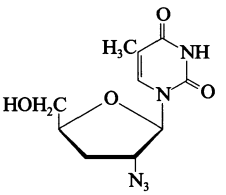
$C_9H_{10}IN_5O_4$ M 379.1

Solid. Mp 152-154°.

Warshaw, J.A. *et al, J. Med. Chem.*, 1990, **33**, 1663 (*synth, ir, pmr, uv*)

2′-Azido-2′,3′-dideoxy-5-methyluridine A-1-00253

[126543-51-9]



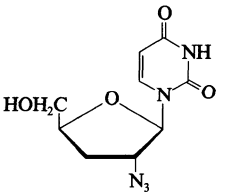
$C_{10}H_{13}N_5O_4$ M 267.2

Solid. Mp 167-169°. Regioisomer of Zidovudine, A-0-04712.

Warshaw, J.A. *et al, J. Med. Chem.*, 1990, **33**, 1663 (*synth, ir, pmr, uv*)

2′-Azido-2′,3′-dideoxyuridine A-1-00254

[126543-45-1]



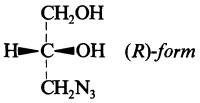
$C_9H_{11}N_5O_4$ M 253.2

Cryst. (EtOH). Mp 167-169°.

Warshaw, J.A. *et al, J. Med. Chem.*, 1990, **33**, 1663 (*synth, pmr, ir, uv*)

3-Azido-1,2-propanediol, 9CI A-1-00255

[73018-98-1]



$C_3H_7N_3O_2$ M 117.1

(R)-form [131321-84-1]

$[\alpha]_D^{20}$ +2.24 (c, 0.5 in $CHCl_3$).

(S)-form [85820-84-4]

Oil.

(±)-form [121651-55-6]

Oil. $Bp_{0.04}$ 86°.

Holý, A., *Coll. Czech. Chem. Comm.*, 1989, **54**, 446 (*synth*)

Ching-Yun, H. *et al, Tetrahedron: Asymmetry*, 1990, **1**, 219 (*R-form*)

Martin, S.F. *et al, J.O.C.*, 1994, **59**, 4821 (*synth, ir, pmr, cmr*)

2-Azidoselenophene A-1-00256

$C_4H_3N_3Se$ M 172.0

Unstable oil.

Gronowitz, S. *et al, J.C.S. Perkin 2*, 1994, 1815.

3-Azidoselenophene A-1-00257

$C_4H_3N_3Se$ M 172.0

Oil.

Gronowitz, S. *et al, J.C.S. Perkin 2*, 1994, 1815.

2-Azido-3-thiophenecarboxaldehyde A-1-00258

2-Azido-3-formylthiophene

[163079-30-9]

$C_5H_3N_3OS$ M 153.1

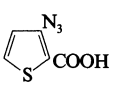
Solid. Mp 80-81° dec. Unstable.

▶ Toxic.

Capperucci, A. *et al, J.O.C.*, 1995, **60**, 2254 (*synth, pmr, ir, cmr*)

3-Azido-2-thiophenecarboxylic acid A-1-00259

[56488-92-7]



$C_5H_3N_3O_2S$ M 169.1

Mp 110° dec.

Me ester:

$C_6H_5N_3O_2S$ M 183.1 Needles (MeOH aq.). Mp 67-68°.

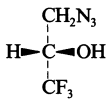
Nitrile: [56488-94-9]. *3-Azido-2-cyanothiophene*

$C_5H_2N_4S$ M 150.1 Cryst. (MeOH). Mp 77.5-79°.

Gronowitz, S. *et al, Acta Chem. Scand., Ser. B*, 1975, **29**, 224.

Dyall, L.K. *et al, J.C.S. Perkin 2*, 1994, 2115.

1-Azido-3,3,3-trifluoro-2-propanol A-1-00260



$C_3H_4F_3N_3O$ M 155.0

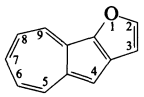
(S)-form [160595-62-0]

$[\alpha]_D^{24}$ +12.89 (c, 1.9 in MeOH) (96% ee).

Ramachandran, P.V. *et al, J.O.C.*, 1995, **60**, 41 (*synth, ir, pmr, cmr, F-19 nmr*)

Azuleno[1,2-*b*]furan A-1-00261

[92798-12-4]



$C_{12}H_8O$ M 168.1

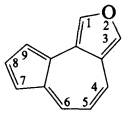
Bluish-green needles. Mp 63-64°.

Fujimori, K. *et al, Chem. Lett.*, 1986, 1021 (*synth, pmr, cmr, uv*)

Yamaguchi, H. *et al, Spectrochim. Acta*, 1987, **43**, 1377.

Azuleno[4,5-*c*]furan A-1-00262

[51273-19-9]



$C_{12}H_8O$ M 168.1

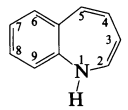
Not isol.

Masaru, S. *et al, Chem. Comm.*, 1983, 1025.

B

1*H*-1-Benzazepine B-1-00001

[264-54-0]



$C_{10}H_9N$ M 143.1

N-*Ac:* [76056-09-2].
$C_{12}H_{11}NO$ M 185.2 Oil.

N-*Benzoyl:* [74422-10-9].
$C_{17}H_{13}NO$ M 247.2 Oil.

N-*Et:*
$C_{12}H_{13}N$ M 171.2 Oil. $Bp_{1.7}$ 89-90°. n_D^{20} 1.5481.

N-*Et, hydrochloride:* Prisms (MeOH). Mp 136-138°.

N-*Benzyl:* [76056-14-9].
$C_{17}H_{15}N$ M 233.3 Oil.

2,3-Dihydro: [3749-12-0].
$C_{10}H_{11}N$ M 145.2 Waxy solid. Mp 48°.

2,3-Dihydro, N-*Ac:* [19673-40-6].
$C_{12}H_{13}NO$ M 187.2 Prisms. Mp 66°.

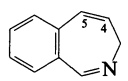
2,3-Dihydro, N-(*4-methylbenzenesulfonyl*): Needles. Mp 108° (EtOH or petrol).

2,3,4,5-Tetrahydro: see *2,3,4,5-Tetrahydro-1H-1-benzazepine, T-0-00914*

Evans, D. *et al, J.C.S.*, 1965, 4806 (*N-Et*)
Hannah, E.D. *et al, J.C.S.(C)*, 1968, 1280 (*dihydro*)
Ikeda, M. *et al, Tet. Lett.*, 1980, **21**, 3403 (*N-derivs, uv, ms*)
Ikeda, M. *et al, J.C.S. Perkin 1*, 1982, 741 (*N-derivs, synth, uv, pmr*)

3*H*-2-Benzazepine, 9CI B-1-00002

[264-20-0]



$C_{10}H_9N$ M 143.1
No phys. props. descr.

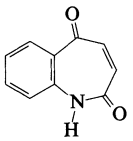
4,5-Dihydro: [23758-95-4].
$C_{10}H_{11}N$ M 145.2 Liq. $Bp_{0.6}$ 85-90°. Readily forms a cryst. dimer. A chloroform soln. of the dimer on standing for several days is slowly converted to the monomer.

4,5-Dihydro, picrate: [23758-96-5]. Yellow cryst. Mp 159-160°.

Goldman, I.M. *et al, J.A.C.S.*, 1969, **91**, 4941 (*dihydro deriv*)
Gomez, P.V. *et al, An. Quim.*, 1974, **70**, 614 (*dihydro, synth, pmr*)
Corriu, R.J.P. *et al, J.O.C.*, 1993, **58**, 1443 (*synth, pmr, cmr, ir*)

1*H*-1-Benzazepine-2,5-dione, 9CI B-1-00003

[10315-38-5]

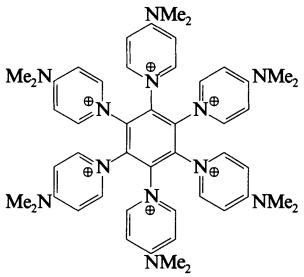


$C_{10}H_7NO_2$ M 173.1
Cryst. Mp 222-223°.

Rickards, R.W. *et al, Tet. Lett.*, 1966, 2361 (*synth, ir, uv, pmr*)
Kozikowski, A.P. *et al, J. Med. Chem.*, 1993, **36**, 2908 (*synth*)

1,1′,1″,1‴,1⁗,1⁗′-(1,2,3,4,5,6-Benzenehexayl)hexakis[4-(dimethylamino)pyridinium] (6+), 9CI B-1-00004

Hexakis(4-dimethylamino-1-pyridinio)benzene



$C_{48}H_{60}N_{12}^{6\oplus}$ M 805.0 (ion)

Hexakis(trifluoromethanesulfonate): [170743-23-4].
$C_{54}H_{60}F_{18}N_{12}O_{18}S_6$ M 1699.5 Cryst. (H_2O). Stable to boiling water, hydrol. by weak base.

Weiss, R. *et al, Angew. Chem., Int. Ed.*, 1995, **34**, 1319 (*synth, ir, pmr, cmr, F-19 nmr, cryst struct*)

Benzenemethanesulfenothioic acid, 9CI B-1-00005

Benzyl hydrodisulfide

[3492-66-8]

$PhCH_2SSH$

$C_7H_8S_2$ M 156.2
Liq. d_4^{20} 1.174. $Bp_{0.1}$ 65-70°. n_D^{20} 1.625.

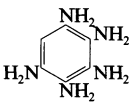
Na salt: [120506-35-6].
Solid.

Tsurugi, J. *et al, J.O.C.*, 1959, **24**, 807 (*synth*)
Kawamura, S. *et al, Bull. Chem. Soc. Jpn.*, 1971, **44**, 2878 (*pmr*)
Mieloszynski, J.L. *et al, Sulfur Lett.*, 1988, **8**, 115 (*synth*)

Benzenepentamine B-1-00006

Pentaaminobenzene

[608-97-9]



$C_6H_{11}N_5$ M 153.1
Brown-black solid or dark brown cryst. (phenylhydrazine). Mp 228° dec. (under H_2). Dec. in air, used immediately.

Praefcke, K. *et al, Annalen*, 1989, 617 (***synth***, *bibl*)

Benzenesulfonyl thiocyanate B-1-00007

Benzene sulfonothioic acid anhydrosulfide with thiocyanic acid, 9CI. Benzenesulfonic thiocyanic anhydride

[1197-98-4]

$PhSO_2SCN$

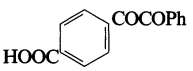
$C_7H_5NO_2S_2$ M 199.2
Cryst. (petrol). Mp 28.5°. Dec. on storage with evolution of SO_2.

Ger. Pat., 1 219 021, (1966); *CA*, **66**, 2368n (*synth*)
Austad, T., *Acta Chem. Scand., Ser. A*, 1975, **29**, 241 (*synth, ir*)
Tanaskov, M.M. *et al, Zh. Org. Khim.*, 1981, **17**, 1800; *J. Org. Chem. USSR (Engl. Transl.)*, 1981, **17**, 1609 (*props*)

Benzil-4-carboxylic acid B-1-00008

4-(Oxophenylacetyl)benzoic acid, 9CI. p-(*Phenylglyoxyloyl*)*benzoic acid, 8CI*

[72857-25-1]



$C_{15}H_{10}O_4$ M 254.2
Cryst. Mp 227-228°.

Me ester: [52380-62-8].
$C_{16}H_{12}O_4$ M 268.2 Cryst. Mp 65-66°.

Kariyone, T. *et al, Yakugaku Zasshi*, 1951, **71**, 926 (*synth*)
Van Es, T. *et al, J.C.S.*, 1963, 1371 (*synth*)

Benzil-3,3′-dicarboxylic acid B-1-00009

3,3′-(1,2-Dioxoethanediyl)bisbenzoic acid, 9CI

[117999-78-7]

$C_{16}H_{10}O_6$ M 298.2

Kim, J.I. *et al, Bull. Korean Chem. Soc.*, 1988, **9**, 30 (*synth, ir, pmr, cmr*)

Benzil-4,4′-dicarboxylic acid B-1-00010

4,4′-(1,2-Dioxoethanediyl)bisbenzoic acid, 9CI. 4,4′-Oxalyldibenzoic acid, 8CI

[1585-67-7]

$C_{16}H_{10}O_6$ M 298.2
Cryst. Mp 324-325°.

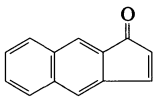
Di-Me ester: [66553-02-4].

$C_{18}H_{14}O_6$ M 326.3 Cryst. Mp 196-197°.

van Es, T. *et al*, *J.C.S.*, 1963, 1371.

1*H*-Benz[*f*]inden-1-one, 9CI B-1-00011

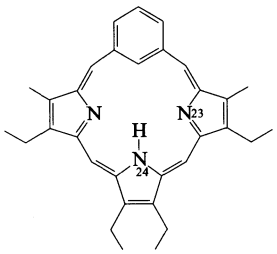
[159113-90-3]



$C_{13}H_8O$ M 180.2
Yellow cryst. by subl.

Morris, J.L. *et al*, *J.O.C.*, 1994, **59**, 6484 (*synth, pmr*)

Benziporphyrin B-1-00012



$C_{32}H_{35}N_3$ M 461.6
Shows tautomerism between the 24*H*- (illus.) and 23*H*-forms. Blue-black cryst. Mp 135-138° dec. The name proposed for the parent skeleton is Benziporphin.

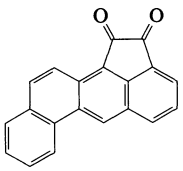
[157643-37-3, 157643-38-4]

Berlin, K. *et al*, *Angew. Chem., Int. Ed.*, 1994, **33**, 1246 (*synth, ir, uv, pmr, cmr*)

Benz[*j*]aceanthrylene-1,2-dione, 9CI B-1-00013

Cholanthrenequinone

[13913-77-4]

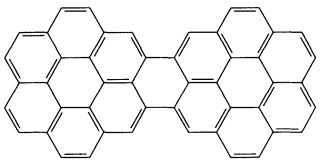


$C_{20}H_{10}O_2$ M 282.2

Miller, D.W. *et al*, *J. Chem. Res., Synop.*, 1984, 418 (*synth, pmr*)

Benzo[1,2,3-*bc*:4,5,6-*b'c'*]dicoronene B-1-00014

Dicoronylene

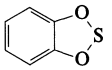


$C_{48}H_{20}$ M 596.6
Incorr. struct. originally assigned. Red needles. Mp >550°. Intense green fluor. in soln.

Zander, M. *et al*, *Chem. Ber.*, 1958, **91**, 2794 (*synth*)
Goddard, R. *et al*, *J.A.C.S.*, 1995, **117**, 30 (*struct*)

1,3,2-Benzodioxathiole, 9CI B-1-00015

[274-17-9]



$C_6H_4O_2S$ M 140.1

S-*Oxide:* [6255-58-9]. *Pyrocatechol cyclic sulfite, 8CI. Catechol sulfite.* o-*Phenylene sulfite*
$C_6H_4O_3S$ M 156.1 Pale yellow liq. Bp_{105} 137-138°, $Bp_{1.5}$ 58°.

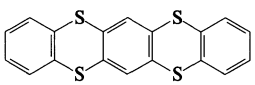
S,S-*Dioxide:* [4074-55-9]. *Pyrocatechol cyclic sulfate, 8CI. Catechol sulfate.* o-*Phenylene sulfate*
$C_6H_4O_4S$ M 172.1 Needles (hexane or by subl.). Mp 35.5-36°.

Green, A.L., *J.C.S.*, 1927, 500 (*oxide*)
Denivelle, L., *C. R. Hebd. Seances Acad. Sci.*, 1936, **203**, 194 (*dioxide*)
Boer, F.P. *et al*, *J.A.C.S.*, 1969, **91**, 6604 (*dioxide, cryst struct*)
De Jongh, D.C. *et al*, *J.O.C.*, 1972, **37**, 1129 (*oxides, synth, ms, ir*)
DuBois, G.E. *et al*, *J.O.C.*, 1980, **45**, 5371 (*dioxide*)
Tickner, A.M. *et al*, *Synth. Commun.*, 1994, **24**, 1631 (*dioxide, synth, ir, pmr, cmr*)

[1,4]Benzodithiino[2,3-*b*]thianthrene, 9CI B-1-00016

5,7,12,14-Tetrathiapentacene

[52879-14-8]



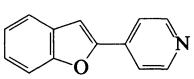
$C_{18}H_{10}S_4$ M 354.5
Cryst. Mp 325°.

Ziegler, M. *et al*, *Chem.-Ztg.*, 1976, **100**, 195 (*synth, ms, ir, pmr, epr*)
Marti, C. *et al*, *J.O.C.*, 1994, **59**, 6200 (*synth, pmr, epr*)

4-(2-Benzofuranyl)pyridine, 9CI B-1-00017

2-(4-Pyridyl)benzofuran. ***Pyridarone, INN.*** *L4269-Labaz*

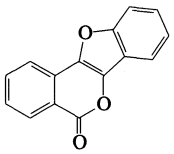
[7035-04-3]



$C_{13}H_9NO$ M 195.2
Anxiolytic, tranquilliser. Never marketed. Cryst. (petrol). Mp 133-134°.

Netherlands Pat., 6 514 447, (1966) (*Soc Belge de l'Azote*); *CA*, **65**, 10570a (*synth*)
Ziegler, H.J. *et al*, *Eur. J. Med. Chem.* (*Chim. Ther.*), 1971, **6**, 159 (*synth, pharmacol*)
Swiss Pat., 613 451, (1979) (*Ciba-Geigy*); *CA*, **92**, 6428s (*synth*)

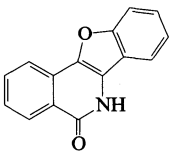
5*H*-Benzofuro[3,2-*c*][2]-benzopyran-5-one B-1-00018



$C_{15}H_8O_3$ M 236.2
Cryst. (C_6H_6). Mp 168-169°.

Yamaguchi, S. *et al*, *J. Het. Chem.*, 1995, **32**, 419 (*synth, uv, cmr*)

Benzofuro[3,2-*c*]isoquinolino-5(6*H*)-one B-1-00019

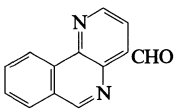


$C_{15}H_9NO_2$ M 235.2
Cryst. (EtOH). Mp 310°.

Yamaguchi, S. *et al*, *J. Het. Chem.*, 1995, **32**, 419 (*synth, uv, cmr*)

Benzo[*c*][1,5]naphthyridine-4-carboxaldehyde B-1-00020

4-Formylbenzo[c][*1,5*]*naphthyridine*

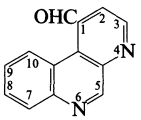


$C_{13}H_8N_2O$ M 208.2
Small cryst. (cyclohexane). Mp 140-141°.

Chrzastek, L. *et al*, *Aust. J. Chem.*, 1994, **47**, 2129 (*synth, pmr*)

Benzo[*f*][1,7]naphthyridine-1-carboxaldehyde B-1-00021

1-Formylbenzo[f][*1,7*]*naphthyridine*



$C_{13}H_8N_2O$ M 208.2
Small cryst. (cyclohexane). Mp 269-270°.

Chrzastek, L. *et al*, *Aust. J. Chem.*, 1994, **47**, 2129 (*synth, pmr*)

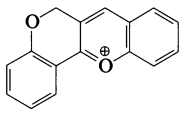
Benzo[*f*][1,7]naphthyridine-3-carboxaldehyde B-1-00022

3-Formylbenzo[f][*1,7*]*naphthyridine*

$C_{13}H_8N_2O$ M 208.2
Small cryst. (cyclohexane). Mp 246-247°.

Chrzastek, L. *et al, Aust. J. Chem.*, 1994, **47**, 2129 (*synth, pmr*)

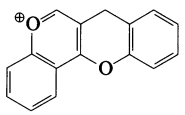
6*H*-[1]Benzopyrano[4,3-*b*][1]benzopyrylium(1+), 9CI B-1-00023



$C_{16}H_{11}O_2^{\oplus}$ M 235.2 (ion)
Perchlorate: [28658-13-1].
$C_{16}H_{11}ClO_6$ M 334.7 Red powder. Mp 234° dec.

Andrieux, J. *et al, Bull. Soc. Chim. Fr.*, 1973, 3421 (*synth, pmr*)
Dean, F.M. *et al, J.C.S. Perkin 1*, 1993, 2675 (*synth, uv, pmr*)

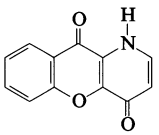
7*H*-1-Benzopyrano[3,2-*c*]benzopyrylium(1+), 9CI B-1-00024



$C_{16}H_{11}O_2^{\oplus}$ M 235.2 (ion)
Perchlorate: [153650-26-1].
$C_{16}H_{11}ClO_6$ M 334.7 Yellow flakes. Mp 207° dec.

Dean, F.M. *et al, J.C.S. Perkin 1*, 1993, 2675 (*synth, uv, pmr*)

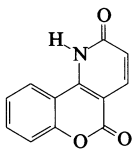
1*H*-Benzopyrano[3,2-*b*]pyridine-4,10-dione B-1-00025



$C_{12}H_7NO_3$ M 213.1
Solid by subl. Mp >260°. Subl.$_3$ 190°.

Mongin, O. *et al, J.C.S. Perkin 1*, 1995, 2503 (*synth, ir, pmr, cmr*)

2*H*-[1]Benzopyrano[4,3-*b*]pyridine-2,5(1*H*)-dione B-1-00026



$C_{12}H_7NO_3$ M 213.1

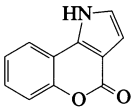
N-*Me:*
$C_{13}H_9NO_3$ M 227.2 Cryst. (EtOH). Mp 210-212°.

N-*Et:*
$C_{14}H_{11}NO_3$ M 241.2 Cryst. (EtOH). Mp 192-193°.

N-*Benzyl:*
$C_{19}H_{13}NO_3$ M 303.3 Mp 203-204° (199°).

Heber, D. *et al, J. Het. Chem.*, 1995, **32**, 505.

[1]Benzopyrano[4,3-*b*]pyrrol-4(1*H*)-one, 9CI B-1-00027



$C_{11}H_7NO_2$ M 185.1
Cryst. (MeOH). Mp 289-291°.

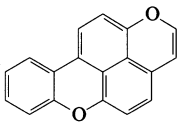
N-*Me:* [85175-18-4].
$C_{12}H_9NO_2$ M 199.2 Cryst. (MeOH). Mp 164-165° (158°).

N-*Ph:* [85175-17-3].
$C_{17}H_{11}NO_2$ M 261.2 Cryst. (MeOH). Mp 143°.

Eiden, F. *et al, Annalen*, 1983, 165 (*N-Me, N-Ph, synth*)
González, A. *et al, Synthesis*, 1994, 279 (*synth, pmr, cmr*)

1-Benzopyrano[6,5,4-*mna*]xanthene B-1-00028

1,6-Dioxabenzo[a]*pyrene*



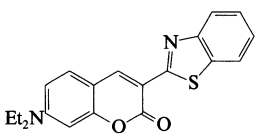
$C_{18}H_{10}O_2$ M 258.2
Pale yellow cryst. (pentane). Mp 139-140°.

Buisson, J.P. *et al, J. Het. Chem.*, 1995, **32**, 17 (*synth, uv, pmr, cmr*)

3-(2-Benzothiazolyl)-7-(diethylamino)-2*H*-1-benzopyran-2-one, 9CI B-1-00029

3-(2-Benzothiazolyl)-7-(diethylamino) coumarin. Coumarin 540. Coumarin 6

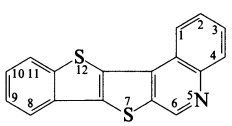
[38215-36-0]



$C_{20}H_{18}N_2O_2S$ M 350.4
Laser dye. Orange needles (Py aq.). Mp 204°.

UK Pat., 867 592, (1961); *CA*, **55**, 21927c (*synth, uv*)
Jasinski, J.P. *et al, Acta Cryst. C*, 1995, **51**, 531 (*cryst struct, bibl*)

[1]Benzothieno[2′,3′:4,5]thieno[2,3-*c*]quinoline B-1-00030



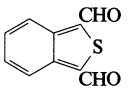
$C_{17}H_9NS_2$ M 291.3

Cryst. (C_6H_6). Mp 220-221°.

Luo, J. *et al, J. Het. Chem.*, 1995, **32**, 659 (*synth, pmr, cmr*)

Benzo[*c*]thiophene-1,3-dicarboxaldehyde, 9CI B-1-00031

[147807-93-0]



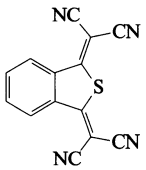
$C_{10}H_6O_2S$ M 190.2
Yellow brown cryst. (hexane/$CHCl_3$). Mp 161-163°.

Lorcy, D. *et al, Chem. Comm.*, 1993, 345 (*synth, uv, pmr, ir*)

2,2′-(Benzo[*c*]thiophene-1,3-diylidene)bispropanedinitrile, 9CI B-1-00032

1,3-Dihydro-1,3-bis(dicyanomethylene) isothianaphthene

[147807-91-8]

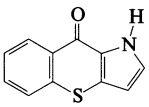


$C_{14}H_4N_4S$ M 260.2
Orange-red cryst. (MeCN). Mp 254°.

Lorcy, D. *et al, Chem. Comm.*, 1993, 345 (*synth, uv, pmr, ir, cryst struct*)

[1]Benzothiopyrano[3,2-*b*]pyrrol-9(1*H*)-one B-1-00033

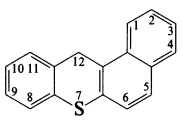
[160205-73-2]



$C_{11}H_7NOS$ M 201.2
Pink cryst. (EtOH). Mp 189-192°.

Bates, D.K. *et al, J.O.C.*, 1994, **59**, 8076 (*synth, ir, pmr*)

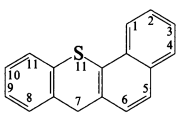
12*H*-Benzo[*a*]thioxanthene B-1-00034



$C_{17}H_{12}S$ M 248.3
Needles (toluene). Mp 109-109.5°.

Takido, T. *et al, J. Het. Chem.*, 1995, **32**, 687 (*synth, pmr*)

7*H*-Benzo[*c*]thioxanthene B-1-00035



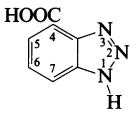
$C_{17}H_{12}S$ M 248.3

Needles (toluene). Mp 88.5-89.5°.

Takido, T. *et al*, *J. Het. Chem.*, 1995, **32**, 687 (*synth, pmr*)

1*H*-Benzotriazole-4(7)-carboxylic acid B-1-00036

[62972-61-6]



$C_7H_5N_3O_2$ M 163.1

Hoffmann, H. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1989, **322**, 457 (*synth*)

1*H*-Benzotriazole-5(6)-carboxylic acid B-1-00037

[23814-12-2]

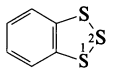
$C_7H_5N_3O_2$ M 163.1
Mp 310° dec. pK_a 4.03 (20°).

Me ester: [113053-50-2].
$C_8H_7N_3O_2$ M 177.1 Cryst. (H_2O). Mp 170-171°.

Et ester: [73605-91-1].
$C_9H_9N_3O_2$ M 191.1 Cryst. (H_2O). Mp 108-109°.

Gilbert, E.E., *J. Het. Chem.*, 1969, **6**, 483 (*synth*)
Katritzky, A.R. *et al*, *Synth. Commun.*, 1993, **23**, 2019 (*ester*)

Benzotrithiole, 9CI B-1-00038



$C_6H_4S_3$ M 172.2

1-Oxide: [146953-96-0].
$C_6H_4OS_3$ M 188.2 Cryst. ($CHCl_3$/hexane). Mp 73-74°.

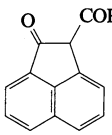
2-Oxide: [36264-19-4].
$C_6H_4OS_3$ M 188.2 Yellow needles ($CHCl_3$/hexane). Mp 76-77°.

Steinle, K. *et al*, *Z. Naturforsch., B*, 1972, **27**, 83 (*synth, ir, pmr, ms*)
Yomoji, N. *et al*, *J.C.S. Perkin 1*, 1993, 1995 (*synth, ir, pmr, cmr*)

2-Benzoyl-1(2*H*)-acenaphthylenone, 9CI B-1-00039

2-Benzoylacenaphthenone

[160771-20-0]



$C_{19}H_{12}O_2$ M 272.3
Yellow needles (hexane). Mp 101-102°.

Tsuge, O. *et al*, *J. Het. Chem.*, 1994, **31**, 1283.

3-Benzoylbenzaldehyde, 9CI B-1-00040

m-*Formylbenzophenone*

[71856-95-6]

$C_{14}H_{10}O_2$ M 210.2
Liq. $Bp_{0.04}$ 140-150°.

Japan. Pat., 79 76 563, (1979); 1980, 80 143 926, 80 162 736, 80 154 932, 80 154 933, 80 154 934; *CA*, **92**, 22259t; **94**, 174660w, 174661x, 174662y; **95**, 61774p, 115075c (*synth*)
Elliott, M. *et al*, *Pestic. Sci.*, 1983, **14**, 182 (*synth, pmr*)

3-Benzoylbenzenesulfonic acid, 9CI B-1-00041

Benzophenone-m-*sulfonic acid*

[63113-58-6]

$C_{13}H_{10}O_4S$ M 262.2
Isol. as the $NH_4^{\oplus}$ and $Ba^{2\oplus}$ salts.

Amide: [134187-86-3].
$C_{13}H_{11}NO_3S$ M 261.3 Needles (H_2O). Mp 144°.

Ruggli, P. *et al*, *Helv. Chim. Acta*, 1941, **24**, 197 (*synth*)

4-Benzoylbenzenesulfonic acid, 9CI B-1-00042

Benzophenone-p-*sulfonic acid*

[73621-00-8]

$C_{13}H_{10}O_4S$ M 262.2
Mp 187-188° (as *S*-benzylthiouronium salt).

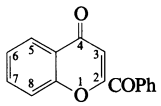
Amide: [28833-72-9].
$C_{13}H_{11}NO_3S$ M 261.3 Cryst. (EtOH). Mp 172-173°.

Bordwell, F.G. *et al*, *J.A.C.S.*, 1956, **78**, 5367 (*synth*)
Dorsett, M.T. *et al*, *J. Med. Chem.*, 1970, **13**, 895 (*synth, amide*)

2-Benzoyl-4*H*-1-benzopyran-4-one, 9CI B-1-00043

2-Benzoylchromone

[51685-51-9]



$C_{16}H_{10}O_3$ M 250.2
Cryst. (EtOH or MeOH). Mp 94°.

Schmutz, J. *et al*, *Helv. Chim. Acta*, 1952, **35**, 1168 (*synth*)
Holmberg, G.-A. *et al*, *Acta Chem. Scand.*, 1973, **27**, 2020 (*synth, ms*)
Payard, M. *et al*, *Eur. J. Med. Chem.* (*Chim. Ther.*), 1981, **16**, 453 (*synth*)

3-Benzoyl-4*H*-1-benzopyran-4-one, 9CI B-1-00044

3-Benzoylchromone

[4197-99-3]

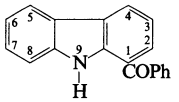
$C_{16}H_{10}O_3$ M 250.2
Cryst. (2-propanol). Mp 130° (125-127°).

Eiden, F. *et al*, *Chem. Ber.*, 1967, **100**, 2554 (*synth, uv*)
Ghosh, C.K. *et al*, *Indian J. Chem., Sect. B*, 1984, **23**, 668 (*synth*)
Adam, W. *et al*, *Annalen*, 1994, 795 (*synth, ir, pmr, cmr*)

1-Benzoylcarbazole B-1-00045

9H-*Carbazol-1-ylphenylmethanone*, *9CI*
Carbazol-1-yl phenyl ketone

[111960-27-1]



$C_{19}H_{13}NO$ M 271.3
Yellow needles (EtOH). Mp 123-125°.

Bonesi, S.M. *et al*, *J. Het. Chem.*, 1991, **28**, 1035 (*synth, pmr, cmr, ms*)

2-Benzoylcarbazole B-1-00046

9H-*Carbazol-2-ylphenylmethanone*, *9CI*

[23592-78-1]

$C_{19}H_{13}NO$ M 271.3
Greenish-yellow plates (AcOH). Mp 163°.

Itier, J. *et al*, *Bull. Soc. Chim. Fr.*, 1969, 2342, 3523 (*synth, ir, uv*)

3-Benzoylcarbazole B-1-00047

9H-*Carbazol-3-ylphenylmethananone*, *9CI*

[19264-66-5]

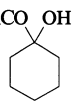
$C_{19}H_{13}NO$ M 271.3
Pale yellow plates (EtOH). Mp 213-215° (203-205°).

Acheson, R.M. *et al*, *J.C.S.*, 1953, 1900 (*synth*)
Itier, J. *et al*, *Bull. Soc. Chim. Fr.*, 1969, 2342, 3523 (*synth, ir, uv*)
Bonesi, S.M. *et al*, *J. Het. Chem.*, 1991, **28**, 1035 (*synth, pmr, cmr, ms, bibl*)

1-Benzoylcyclohexanol B-1-00048

(*1-Hydroxycyclohexyl*)*phenylmethanone*, *9CI*

[947-19-3]



$C_{13}H_{16}O_2$ M 204.2
Cryst. (hexane). Mp 44-44.5°, Mp 48-49°.

Stevens, C.L. *et al*, *J.A.C.S.*, 1952, **74**, 618 (*synth*)
Krepski, L.R. *et al*, *Tet. Lett.*, 1983, **24**, 4075 (*synth*)
Ohta, S. *et al*, *Chem. Pharm. Bull.*, 1995, **43**, 1294 (*synth, pmr*)

Benzoyldiazoacetaldehyde B-1-00049

Benzoylformyldiazomethane

[14762-47-1]

$PhCOC(N_2)CHO$

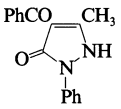
$C_9H_6N_2O_2$ M 174.1
Cryst. (hexane). Mp 60-60.5°.

Stojanovic, F.M. *et al*, *Coll. Czech. Chem. Comm.*, 1967, **32**, 2155.
Sezer, O. *et al*, *Helv. Chim. Acta*, 1994, **77**, 2323.

4-Benzoyl-1,2-dihydro-5-methyl-2-phenyl-3*H*-pyrazol-3-one, 9CI B-1-00050

4-Benzoyl-3-methyl-1-phenyl-5-pyrazolone

[64598-48-7]



$C_{17}H_{14}N_2O_2$ M 278.3

5 Tautomers possible. Crystallises from polar solvs. as the colourless *NH* tautomer (illus.). From non-polar solvs. crystallises as a yellow form of undetd. struct. Shows interesting solvent extraction and complexing props. Mp 91°, Mp 122°.

Jensen, B.S., *Acta Chem. Scand.*, 1959, **13**, 1668, 1890 (*synth, use*)

O'Connell, M.J. *et al*, *Aust. J. Chem.*, 1985, **38**, 401 (*cryst struct*)

Bonati, F. *et al*, *Polyhedron*, 1985, **4**, 357 (*use*)

N-Benzoyl-*N'*-formylhydrazine B-1-00051

Benzoic acid 2-formylhydrazide, 9CI

[28004-69-5]

PhCONHNHCHO

$C_8H_8N_2O_2$ M 164.1

Cryst. (toluene/EtOH). Mp 161-162°.

Carlsen, P.H.J. *et al*, *J. Het. Chem.*, 1994, **31**, 805 (*synth, cmr, pmr, ir*)

(1-Benzoyl-2-oxo-2-phenylethyl) triphenylphosphonium(1+) B-1-00052

(Dibenzoylmethyl)triphenylphosphonium

$Ph_3P^{\oplus}CH(COPh)_2$

$C_{33}H_{26}O_2P^{\oplus}$ M 485.5 (ion)

Perchlorate: [116178-80-4].
$C_{33}H_{26}ClO_6P$ M 584.9 Cryst. (EtOAc/hexane). Mp 185-187°.

Ylide: see *1,3-Diphenyl-2-(triphenylphosphoranylidene)-1,3-propanedione, D-0-12546*

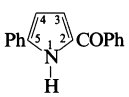
[63634-63-9, 63634-64-0]

Ohmori, H. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 613 (*synth, ir, pmr, use*)

2-Benzoyl-5-phenylpyrrole B-1-00053

Phenyl(5-phenyl-1H-pyrrol-2-yl)methanone, 9CI

[56900-73-3]



$C_{17}H_{13}NO$ M 247.2

Cryst (EtOH). Mp 166°.

Padwa, A. *et al*, *J.A.C.S.*, 1975, **97**, 4682 (*synth, uv, pmr*)

Kharchenko, V.G. *et al*, *Khim. Geterotsikl. Soedin.*, 1984, 1355; 1985, 352; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1984, 1113; 1985, 291 (*synth, cryst struct, ir, pmr*)

Messinger, P. *et al*, *Synthesis*, 1986, 213 (*synth, ir, pmr*)

Pale-Grosdemage, C. *et al*, *Tetrahedron*, 1989, **45**, 3397 (*ir, pmr, cmr, ms*)

3-Benzoyl-4-phenylpyrrole B-1-00054

Phenyl(4-phenyl-1H-pyrrol-3-yl)methanone, 9CI

[40167-32-6]

$C_{17}H_{13}NO$ M 247.2

Cryst. (CH_2Cl_2). Mp 232-234°.

van Leusen, A.M. *et al*, *Tet. Lett.*, 1972, 5337 (*synth*)

van Leusen, D. *et al*, *J.O.C.*, 1992, **57**, 2245 (*synth, ir, pmr*)

3-Benzoyl-5-phenylpyrrole B-1-00055

Phenyl(5-phenyl-1H-pyrrol-3-yl)methanone, 9CI

[161958-60-7]

$C_{17}H_{13}NO$ M 247.2

Cryst. (DMF aq.). Mp 220-222°.

Di Santo, R. *et al*, *Synth. Commun.*, 1995, **25**, 795 (*synth*)

4-Benzoylpyridazine B-1-00056

Phenyl-4-pyridazinylmethanone, 9CI. Phenyl 4-pyridazinyl ketone

[53074-23-0]

$C_{11}H_8N_2O$ M 184.1

Needles (petrol). Mp 106-108°.

Oxime: [96054-53-4].
$C_{11}H_9N_3O$ M 199.2 Cryst. (EtOH). Mp 146-149°.

[96054-54-5]

Heinisch, G. *et al*, *Monatsh. Chem.*, 1974, **105**, 648; 1979, **110**, 365 (*synth, pmr*)

Heinisch, G. *et al*, *Annalen*, 1985, 167 (*oxime, synth*)

Yamanaka, H. *et al*, *Heterocycles*, 1990, **31**, 895 (*synth, pmr*)

1-Benzoyl-2-pyrrolidinone, 9CI B-1-00057

N-*Benzoyl-γ-butyrolactam*

[2399-66-8]

$C_{11}H_{11}NO_2$ M 189.2

Catalyst for polymerisation of pyrrolidinones. Needles (EtOH or C_6H_6); platelets (H_2O). Mp 92.5° (89-90°).

Kanewskaja, S.J., *Ber.*, 1936, **69**, 266 (*synth*)

Sekiguchi, H. *et al*, *Bull. Soc. Chim. Fr.*, 1960, 1827 (*synth*)

Korte, F. *et al*, *Chem. Ber.*, 1962, **95**, 2444 (*synth*)

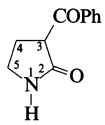
Kato, T. *et al*, *Chem. Pharm. Bull.*, 1979, **27**, 1181 (*synth*)

Sasaki, H. *et al*, *J. Med. Chem.*, 1991, **34**, 628 (*synth, pmr*)

Yamane, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1992, **65**, 886 (*cryst struct*)

3-Benzoyl-2-pyrrolidinone, 9CI B-1-00058

[92288-11-4]



$C_{11}H_{11}NO_2$ M 189.2

Prob. enolised β-diketone. Cryst. (C_6H_6). Mp 122-123° (120°).

N-*Me:* [54343-55-4].
$C_{12}H_{13}NO_2$ M 203.2 Oil. Bp_5 164-165°, $Bp_{0.1}$ 125°.

Korte, F. *et al*, *Chem. Ber.*, 1962, **95**, 2444 (*synth, uv, ir*)

Stehlíček, J. *et al*, *Makromol. Chem.*, 1986, **187**, 513 (*synth, pmr, ms, ir*)

5-Benzoyl-2-pyrrolidinone, 9CI B-1-00059

$C_{11}H_{11}NO_2$ M 189.2

(±)-***form*** [111556-29-7]

Cryst. (MeOH). Mp 175°.

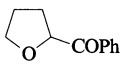
N-*Me:* [42435-96-1].
$C_{12}H_{13}NO_2$ M 203.2 Mp 115°.

Soai, K. *et al*, *J.C.S. Perkin 1*, 1987, 1465 (*synth, pmr, ir*)

Rigo, B. *et al*, *Synth. Commun.*, 1994, **24**, 2597 (*synth, pmr*)

2-Benzoyltetrahydrofuran B-1-00060

Phenyl tetrahydrofuran-2-yl ketone



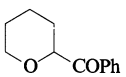
$C_{11}H_{12}O_2$ M 176.2

Oil.

Enholm, E.J. *et al*, *J. Het. Chem.*, 1995, **32**, 109.

2-Benzoyltetrahydro-2*H*-pyran B-1-00061

Phenyltetrahydro-2H-pyran-2-yl ketone



$C_{12}H_{14}O_2$ M 190.2

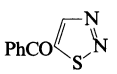
Oil.

Enholm, E.J. *et al*, *J. Het. Chem.*, 1995, **32**, 109 (*synth, pmr, cmr*)

5-Benzoyl-1,2,3-thiadiazole B-1-00062

Phenyl-1,2,3-thiadiazol-5-ylmethanone, 9CI

[136918-89-3]



$C_9H_6N_2OS$ M 190.2

Solid (EtOH). Mp 80°.

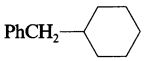
L'abbé, G. *et al*, *J.C.S. Perkin 1*, 1992, 1755 (*synth, ir, pmr, cmr, ms*)

L'abbé, G. *et al*, *J. Het. Chem.*, 1993, **30**, 301 (*N-15 nmr*)

Benzylcyclohexane B-1-00063

(Cyclohexylmethyl)benzene, 9CI. Cyclohexylphenylmethane, 8CI

[4410-75-7]



$C_{13}H_{18}$ M 174.2
Bp 240-241°, Bp_{20} 137°, Bp_{10} 133°.

Rosenmund, K.W. *et al, Chem. Ber.*, 1959, **92**, 494 (*synth*)
Gutsche, C.D. *et al, Tetrahedron*, 1962, **18**, 617 (*synth*)
Tomioka, H. *et al, Tetrahedron*, 1985, **41**, 1435 (*pmr*)
Krafft, M.E. *et al, J.O.C.*, 1988, **53**, 3158 (*synth*)

Benzyl dichloromethyl sulfide B-1-00064

$PhCH_2SCHCl_2$

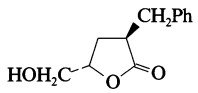
$C_8H_8Cl_2S$ M 207.1
Liq.

S,S-*Dioxide:* [10038-09-2]. *Benzyl dichloromethyl sulfone*
$C_8H_8Cl_2O_2S$ M 239.1 Plates (cyclohexane). Mp 104°.

Paquette, L.A. *et al, J.A.C.S.*, 1967, **89**, 4487 (*synth, deriv*)
Langler, R.F. *et al, Aust. J. Chem.*, 1994, **47**, 1641 (*sulfone*)

3-Benzyldihydro-5-(hydroxymethyl)-2(3*H*)-furanone B-1-00065

Dihydro-5-(hydroxymethyl)-3-(phenylmethyl)-2(3H)-furanone



$C_{12}H_{14}O_3$ M 206.2

(3R,5S)-form
Solid. $[\alpha]_D^{22}$ −2.22 (c, 0.006 in $CHCl_3$).

O-*(Trifluoromethanesulfonyl):* Waxy solid. Mp 53-54°.

Dorsey, B.D. *et al, J. Med. Chem.*, 1994, **37**, 3443 (*synth, ir, pmr, cmr*)

2-Benzyl-1,3-diphenyl-2-propanol B-1-00066

α,α-Bis(phenylmethyl)benzeneethanol, 9CI. Tribenzylmethanol

[6712-97-6]

$(PhCH_2)_3COH$

$C_{22}H_{22}O$ M 302.4
Cryst. (EtOH). Mp 114-115°.

Klages, A. *et al, Ber.*, 1904, **37**, 1447 (*synth*)
Ferguson, G. *et al, Acta Cryst. C*, 1993, **49**, 820 (*cryst struct*)
Ferguson, G. *et al, J. Organomet. Chem.*, 1994, **464**, 95 (*pmr*)

Benzyl ethyl disulfide B-1-00067

Ethyl phenylmethyl disulfide

[21230-16-0]

$PhCH_2—S—S—Et$

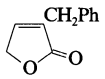
$C_9H_{12}S_2$ M 184.3
Liq. $Bp_{0.1}$ 75°. n_D^{25} 1.5820.

Stirling, C.J.M., *J.C.S.*, 1957, 3597.

3-Benzyl-2(5*H*)-furanone B-1-00068

3-(Phenylmethyl)-2(5H)-furanone, 9CI

[46201-15-4]



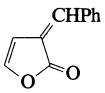
$C_{11}H_{10}O_2$ M 174.1
Oil. $Bp_{0.2}$ 114°, $Bp_{0.01}$ 141-143°.

Canonne, P. *et al, Tet. Lett.*, 1983, **24**, 1929 (*synth*)
Muraoka, O. *et al, J.C.S. Perkin 1*, 1994, 1833 (*synth*)

3-Benzylidene-2(3*H*)-furanone B-1-00069

3-(Phenylmethylene)-2(3H)-furanone, 9CI. Isoaurone

[4645-16-3]



$C_{11}H_8O_2$ M 172.1

[105262-74-6]

Näsman, J.H. *et al, Tet. Lett.*, 1986, **27**, 1391 (*synth*)

Benzyl phenyl disulfide, 8CI B-1-00070

Phenyl phenylmethyl disulfide

[16601-17-5]

$PhCH_2—S—S—Ph$

$C_{13}H_{12}S_2$ M 232.3
Liq. $Bp_{0.05}$ 125-128°.

Jacini, G. *et al, Gazz. Chim. Ital.*, 1952, **82**, 297.

P-Benzylphosphonous diamide B-1-00071

P-*(Phenylmethyl)phosphonous diamide*

$PhCH_2P(NH_2)_2$

$C_7H_{11}N_2P$ M 154.1

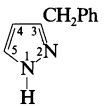
N,N,N′,N′-*Tetra-Et:* [93633-48-8]. *Benzylphosphonous bis(diethylamide). N,N,N′,N′-Tetraethyl-P-(phenylmethyl) phosphonous diamide*
$C_{15}H_{27}N_2P$ M 266.3 Oil. $Bp_{0.02}$ 67°.

Vierling, P. *et al, Organometallics*, 1986, **5**, 2543 (*synth, ir, pmr, P-31 nmr*)

3(5)-Benzyl-1*H*-pyrazole B-1-00072

3-(Phenylmethyl)pyrazole

[32251-82-4]



$C_{10}H_{10}N_2$ M 158.2
Oil. $Bp_{0.05}$ 140-150°. n_D^{20} 1.5762.

Picrate: [32251-83-5].
Yellow cryst. (EtOH/petrol). Mp 125-127°.

Schweizer, E.E. *et al, J.O.C.*, 1971, **36**, 4033 (*synth, ir, pmr*)

4-Benzyl-1*H*-pyrazole B-1-00073

4-(Phenylmethyl)-1H-pyrazole, 9CI

[66948-38-7]

$C_{10}H_{10}N_2$ M 158.2
Cryst. Mp 79-80°.

Oxalate: Cryst. ($EtOH/Et_2O$). Mp 150-151° dec.

N-*Me:* [148873-29-4]. *4-Benzyl-1-methyl-1H-pyrazole*
$C_{11}H_{12}N_2$ M 172.2 Oil.

N-*Me, picrate:* Cryst. Mp 87-89°.

[149507-57-3]

Tolf, B.R. *et al, Acta Chem. Scand., Ser. B*, 1982, **36**, 101 (*synth*)
Echevarria, A. *et al, J.C.S. Perkin 1*, 1993, 2229 (*synth, pmr*)
Echevarria, A. *et al, Synth. Commun.*, 1993, **23**, 925.

4-Benzylpyridazine B-1-00074

4-(Phenylmethyl)pyridazine, 9CI

[53074-22-9]

$C_{11}H_{10}N_2$ M 170.2
Liq. $Bp_{0.001}$ 125°.

Hydrochloride: [53074-25-2].
Cryst. ($EtOH/Et_2O$). Mp 129°.

Heinisch, G. *et al, Monatsh. Chem.*, 1974, **105**, 648 (*synth, pmr*)
Pittenauer, E. *et al, Org. Mass Spectrom.*, 1991, **26**, 595 (*ms*)

5-Benzylpyrimidine B-1-00075

5-(Phenylmethyl)pyrimidine, 9CI

[92674-39-0]

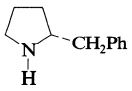
$C_{11}H_{10}N_2$ M 170.2
Cryst. Mp 47°. $Subl._{0.01}$ 60-65°.

Robba, M. *et al, Bull. Soc. Chim. Fr.*, 1960, 1648 (*synth*)

2-Benzylpyrrolidine B-1-00076

2-(Phenylmethyl)pyrrolidine, 9CI

[35840-91-6]



(R)-form

$C_{11}H_{15}N$ M 161.2

(R)-form [63328-13-2]
Oil. Bp_4 95-98°. $[\alpha]_D^{25}$ −15.1 (c, 0.6 in MeOH).

Hydrochloride: [144889-08-7].
Mp 109-111°. $[\alpha]_D$ −33.6 (c, 1.1 in MeOH).

(S)-form [97522-31-1]
Oil. $[\alpha]_D$ +20.0 (c, 0.3 in MeOH).

(±)-form [97589-59-8]
Oil. Bp_{19} 129-131°.

Picrate: [106366-41-0].
Cryst. (EtOH). Mp 136-137°.

N-*Me:* [3211-56-1].
$C_{12}H_7N$ M 165.1 Liq. Bp_{10} 107-108°.

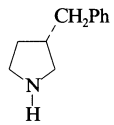
[4266-03-9]

Starr, D.F. *et al, J.A.C.S.*, 1932, **54**, 3971 (*synth*)
Červinka, O., *Coll. Czech. Chem. Comm.*, 1965, **30**, 2403 (*N-Me*)
Tseng, C.C. *et al, Chem. Pharm. Bull.*, 1977, **25**, 29 (*synth, ir, pmr*)
Secor, H.V. *et al, Heterocycles*, 1986, **24**, 1687 (*synth, pmr, cmr*)

Meyers, A.I. *et al*, *J.O.C.*, 1991, **56**, 2294; 1992, **57**, 1656 (*S-form, synth, pmr, cmr*)
Cooper, G.F. *et al*, *Tet. Lett.*, 1992, **33**, 5895 (*R-form, synth*)
Gooding, O.W. *et al*, *Synth. Commun.*, 1995, **25**, 1155 (*R-form, synth*)

3-Benzylpyrrolidine B-1-00077

3-(Phenylmethyl)pyrrolidine, 9CI



(*R*)-*form*

$C_{11}H_{15}N$ M 161.2

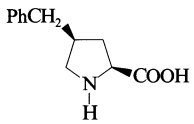
(***R*)-*form*** [155627-32-0]
$[\alpha]_D$ +19.1 (c, 1.5 in EtOH).

(***S*)-*form*** [155627-31-9]
$[\alpha]_D$ −18.2 (c, 1.5 in EtOH).

Westrum, L.J. *et al*, *Tet. Lett.*, 1994, 973 (*synth*)

4-Benzyl-2-pyrrolidinecarboxylic acid B-1-00078

4-Benzylproline



$C_{12}H_{15}NO_2$ M 205.2

(***2S,4S*)-*form***
(−)-cis-*form*
Solid. Mp 190° dec. $[\alpha]_D$ −39.3 (c, 0.28 in MeOH).

Ezquerra, J. *et al*, *J.O.C.*, 1995, **60**, 2925 (*synth, ir, pmr, cmr*)

2,2′-Biadamantyl ketone B-1-00079

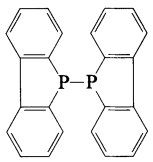
Bis(tricyclo[3.3.1.1^{3,7}]dec-2-yl)methanone, 9CI. 2,2′-Diadamantyl ketone

$C_{21}H_{30}O$ M 298.4
Mp 182° (177.5-179.5°).

Molle, G. *et al*, *J.O.C.*, 1982, **47**, 4120 (*synth*)

5,5′-Bi-(5*H*-benzo[*b*]phosphole), 9CI B-1-00080

[4762-79-2]



$C_{24}H_{16}P_2$ M 366.3
Yellow cryst. Mp 230°.

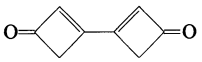
5,5′-Disulfide:
$C_{24}H_{16}P_2S_2$ M 430.4 Complexes with Sm. Pale yellow solid.

Wilson, W.L. *et al*, *Bull. Soc. Chim. Fr.*, 1993, **130**, 673 (*disulfide, pmr, cmr, P-31 nmr*)
Nief, F. *et al*, *J. Organomet. Chem.*, 1994, **464**, 149 (*synth, pmr, P-31 nmr, ms*)

[Bi-1-cyclobuten-1-yl]-3,3′-dione, 9CI B-1-00081

3,3′-Bi(2-cyclobuten-1-one)

[159557-92-3]

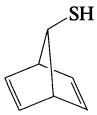


$C_8H_6O_2$ M 134.1
Light yellow solid. Mp 75-260° (slow dec.).

Liebeskind, L.S. *et al*, *J.O.C.*, 1994, **59**, 7917 (*synth, ir, pmr, cmr*)

Bicyclo[2.2.1]hepta-2,5-diene-7-thiol B-1-00082

7-Mercaptonorbornane. 7-Thionorbornadiene



C_7H_8S M 124.2

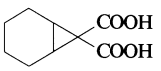
S-*Me:* [136708-44-6]. *7-(Methylthio) bicyclo[2.2.1]hepta-2,5-diene. 7-Methylthionorbornadiene*
$C_8H_{10}S$ M 138.2 Bp_{18} 78°.

Huda, E. *et al*, *Chem. Ber.*, 1991, **124**, 2879.

Bicyclo[4.1.0]heptane-7,7-dicarboxylic acid B-1-00083

Norcarane-7,7-dicarboxylic acid

[20145-30-6]



$C_9H_{12}O_4$ M 184.1
Sl. brown cryst. Mp 186-188° (176-177°) (decarboxylates).

Di-Me ester: [34916-57-9].
$C_{11}H_{16}O_4$ M 212.2 Yellowish cryst. (MeOH). Mp 87-88.5°.

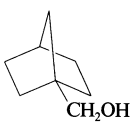
Di-Et ester:
$C_{13}H_{20}O_4$ M 240.2 Mp 36-37°. $Bp_{0.5}$ 108°. n_D^{20} 1.4687.

Musso, H., *Chem. Ber.*, 1968, **101**, 3710 (*synth*)
Ohishi, J., *Synthesis*, 1980, 690 (*synth*)
Troxler, T. *et al*, *Helv. Chim. Acta*, 1994, **77**, 1193 (*synth, pmr, cmr, ms*)

Bicyclo[2.2.1]heptane-1-methanol, 9CI B-1-00084

1-Norbornanemethanol, 8CI. 1-Norcamphanemethanol. 1-Hydroxymethylnorbornane

[2064-02-0]



$C_8H_{14}O$ M 126.1
Waxy needles. Mp 63-65°.

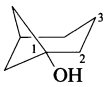
4-Methylbenzenesulfonyl: [13866-80-3]. Cryst. (hexane). Mp 78-80°.
Me ether: [61192-27-6]. *1-(Methoxymethyl) bicyclo[2.2.1]heptane, 9CI*
$C_9H_{16}O$ M 140.2 Liq.

Bixler, R.L. *et al*, *J.O.C.*, 1958, **23**, 742 (*synth*)
Wiberg, K.B. *et al*, *J.A.C.S.*, 1963, **85**, 3188 (*Ac*)
Applequist, D.E. *et al*, *J.A.C.S.*, 1965, **87**, 2194 (*synth*)
Kropp, P.J. *et al*, *J.A.C.S.*, 1976, **98**, 8135 (*Me ether*)
Neuman, R.C. *et al*, *J.O.C.*, 1990, **55**, 4564 (*synth, pmr, cmr*)
Kostova, K. *et al*, *Synth. Commun.*, 1995, **25**, 1575 (*synth, ir, pmr, cmr, ms*)

Bicyclo[3.1.1]heptan-1-ol, 9CI B-1-00085

1-Norpinanol

[130775-52-9]



$C_7H_{12}O$ M 112.1
Cryst. Mp 94-95°, Mp 113-115°.

Razus, A.C. *et al*, *Rev. Roum. Chim.*, 1989, **34**, 2075 (*synth, ir, pmr, cmr*)
Molander, G.A. *et al*, *J.O.C.*, 1991, **56**, 4112 (*synth, pmr, cmr, ms*)

Bicyclo[3.1.1]heptan-2-ol, 9CI B-1-00086

2-Norpinanol, 8CI

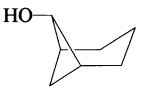
[38102-34-0]

$C_7H_{12}O$ M 112.1

(±)-***form***
Cryst. Mp 101-102°. Sublimes.

Grychtol, K. *et al*, *Chem. Ber.*, 1972, **105**, 1798 (*synth, ir, pmr*)
Bentley, T.W. *et al*, *Annalen*, 1995, 599 (*synth, pmr*)

Bicyclo[3.1.1]heptan-6-ol, 9CI B-1-00087



(1*RS*,6*RS*)-*form*

$C_7H_{12}O$ M 112.1

(***1RS,6RS*)-*form***
exo-*form*
Mp 72-78°.

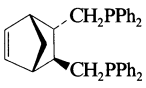
(***1RS,6SR*)-*form*** [6621-22-3]
endo-*form*
Mp 124-126°.

Wiberg, K.B. *et al*, *J.O.C.*, 1966, **31**, 2250 (*synth, pmr*)
Gassman, P.G. *et al*, *J.A.C.S.*, 1981, **103**, 4977 (*synth*)

Bicyclo[2.2.1]hept-5-ene-2,3-diylbis(methylene) bis[diphenylphosphine], 9CI B-1-00088

Updated Entry replacing B-0-01896
2,3-Bis(diphenylphosphinomethyl)-5-norbornene

[128777-26-4]



(2*R**,3*R**)-*form*

$C_{33}H_{32}P_2$ M 490.5
Ligand for asymmetric hydrogenation.

(***2R*,3R**)-*form*** [79426-29-2]
(+)-endo,exo-*form*
Solid. Mp 78-79°. $[\alpha]_D^{25}$ +12.0 (c, 1 in C_6H_6), $[\alpha]_D$ −25.7 (c, 1 in $CHCl_3$).

Dioxide: [79426-27-0].
$C_{33}H_{32}O_2P_2$ M 522.5 Cryst. Mp 204-206°. $[\alpha]_D^{25}$ +77.8 (c, 1 in C_6H_6), $[\alpha]_D$ +33.4 (c, 1 in EtOH), $[\alpha]_D$ +28.2 (c, 1 in $CHCl_3$).

(2S*,3S*)-form [79426-28-1]
(−)-endo,exo-*form*
Solid. Mp 78-79°. $[\alpha]_D^{25}$ −12.1 (c, 1 in C_6H_6), $[\alpha]_D$ +25.2 (c, 1 in $CHCl_3$).

Dioxide: [79426-26-9].
Cryst. Mp 205-206°. $[\alpha]_D^{25}$ −76.4 (c, 1 in C_6H_6), $[\alpha]_D$ −33.4 (c, 1 in EtOH), $[\alpha]_D$ −27.0 (c, 1 in $CHCl_3$).

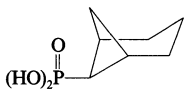
(2RS,3RS)-form [79426-24-7]
(±)-endo,exo-*form*
Solid.

Dioxide: [79426-25-8].
Cryst. (EtOH aq.). Mp 208-209°.

[128777-26-4]

Döbler, C. *et al, J. Prakt. Chem.*, 1981, **323**, 667 (*synth, resoln*)

[Bicyclo[3.1.1]heptyl]-6-phosphonic acid, 9CI B-1-00089



$C_7H_{13}O_3P$ M 176.1

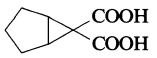
(1α,5α,6β)-form [145852-36-4]
endo-*form*
Cryst. (H_2O). Mp 196-197°.

Di-Me ester: [145852-35-3]. *Dimethyl [bicyclo[3.1.1]heptyl]-6-phosphonate*
$C_9H_{17}O_3P$ M 204.2 Liq. Bp_2 91-92°.

Vasin, V.A. *et al, Zh. Obshch. Khim.*, 1992, **62**, 1416; *J. Gen. Chem. USSR (Engl. Transl.)*, 1992, **62**, 1164 (*synth, ir, ms, pmr, cmr, P-31 nmr*)

Bicyclo[3.1.0]hexane-6,6-dicarboxylic acid B-1-00090

[160002-70-0]



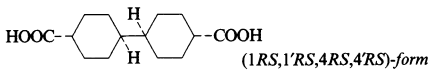
$C_8H_{10}O_4$ M 170.1
Cryst. (H_2O). Mp 190-191° (decarboxylates).

Di-Me ester: [160002-69-7].
$C_{10}H_{14}O_4$ M 198.2 Cryst. (MeOH). Mp 47-48°.

Troxler, T. *et al, Helv. Chim. Acta*, 1994, **77**, 1193 (*synth, pmr, cmr, ms*)

[1,1′-Bicyclohexyl]-4,4′-dicarboxylic acid, 9CI B-1-00091

[1459-29-6]



(*1RS,1′RS,4RS,4′RS*)-*form*

$C_{14}H_{22}O_4$ M 254.3

(1RS,1′RS,4RS,4′RS)-form [16200-85-4]
trans,trans-*form*
Cryst. (AcOH). Mp 351-353° (340°).

Di-Me ester: [16200-84-3].
Needles (MeOH). Mp 115-116°.

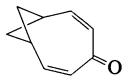
(1RS,1′RS,4SR,4′SR)-form [46902-11-8]
cis,cis-*form*
Mp 260-263°.

Di-Me ester:
$C_{16}H_{26}O_4$ M 282.3 Plates (MeOH). Mp 98°.

Fichter, F. *et al, Helv. Chim. Acta*, 1938, **21**, 141 (*synth*)
Deutscher, H.-J. *et al, Z. Chem.*, 1984, **24**, 257 (*synth*)
Cannon, J.G. *et al, Synth. Commun.*, 1995, **25**, 2079 (*synth, conformn, cryst struct*)

Bicyclo[5.1.1]nona-2,5-dien-4-one, 9CI B-1-00092

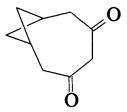
[145325-93-5]



$C_9H_{10}O$ M 134.1
Oil.

Paquette, L.A. *et al, J.O.C.*, 1994, **59**, 5700 (*synth, ir, pmr, cmr*)

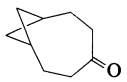
Bicyclo[5.1.1]nonane-3,5-dione B-1-00093



$C_9H_{12}O_2$ M 152.1
Cryst. solid (Et_2O). Mp 98-99°.

Paquette, L.A. *et al, J.O.C.*, 1994, **59**, 5700 (*synth, ir, pmr, cmr*)

Bicyclo[5.1.1]nonan-4-one B-1-00094



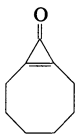
$C_9H_{14}O$ M 138.2
Solid. Mp 89-91°.

Paquette, L.A. *et al, J.O.C.*, 1994, **59**, 5700 (*synth, pmr, ir, cmr*)

Bicyclo[6.1.0]non-1(8)-en-9-one, 8CI B-1-00095

Cyclooctanocyclopropenone. Hexamethylenecyclopropenone

[30493-03-9]



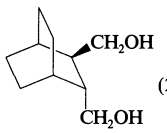
$C_9H_{12}O$ M 136.1
Unstable yellow liq. $Bp_{0.05}$ 110°.

2,4-Dinitrophenylhydrazone: [30493-04-0]. Red solid (EtOH). Mp 198.5-199.5°.

Wittig, G. *et al, Annalen*, 1970, **741**, 79 (*synth, ir, pmr*)
Gleiter, R. *et al, Synthesis*, 1995, 969 (*synth, pmr, cmr*)

Bicyclo[2.2.2]octane-2,3-dimethanol, 9CI B-1-00096

2,3-Bis(hydroxymethyl)bicyclo[2.2.2]octane



(2*R*,3*R*)-*form*

$C_{10}H_{18}O_2$ M 170.2

(2R,3R)-form [57222-03-4]
(+)-trans-*form*
Needles. Mp 111.5°. $[\alpha]_D^{20}$ +101 (c, 0.5 in $CHCl_3$).

(2RS,3RS)-form [65830-47-9]
(±)-trans-*form*
Cryst. Mp 86°.

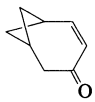
(2RS,3SR)-form [65942-08-7]
cis-*form*
Cryst. Mp 88-89°.

Collet, A. *et al, Bull. Soc. Chim. Fr.*, 1977, 494 (*synth*)
Brouwer, H. *et al, Org. Magn. Reson.*, 1977, **9**, 360 (*cmr*)
Lok, K.P. *et al, J.A.C.S.*, 1985, **107**, 2521 (*synth, pmr*)
Consiglio, G. *et al, Organometallics*, 1991, **10**, 2046 (*synth*)
Waldmann, H. *et al, Helv. Chim. Acta*, 1994, **77**, 2111 (*synth*)

Bicyclo[4.1.1]oct-4-en-3-one, 9CI B-1-00097

Bicyclo[4.1.1]oct-3-en-4-one (incorr.)

[166803-23-2]



$C_8H_{10}O$ M 122.1

(±)-form
Solid. Mp 38.5-39.5°. $Bp_{1.5}$ 35-40° (bulb).

Paquette, L.A. *et al, J.O.C.*, 1994, **59**, 5700 (*synth, pmr, cmr*)

Bicyclo[1.1.1]pentane-1-thiol B-1-00098

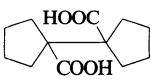
1-Mercaptobicyclo[1.1.1]pentane

C_5H_8S M 100.1

S-*Ph:* [98585-81-0]. *1-(Phenylthio) bicyclo[1.1.1]pentane, 9CI*
$C_{11}H_{12}S$ M 176.2 Liq.

Semmler, K. *et al, J.A.C.S.*, 1985, **107**, 6410 (*S-Ph, synth, pmr, cmr*)
Wiberg, K.B. *et al, J.A.C.S.*, 1990, **112**, 2194 (*S-Ph, synth, pmr*)
Toops, D.S. *et al, J.O.C.*, 1993, **58**, 6505 (*S-Ph, synth*)

[1,1′-Bicyclopentyl]-1,1′-dicarboxylic acid, 9CI B-1-00099



$C_{12}H_{18}O_4$ M 226.2

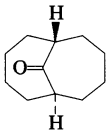
Cryst. (AcOH aq. or MeOH). Mp 202-204° (157-158.5°, 170-174°). pK_{a1} 5.87; pK_{a2} 9.83 (20°, 50% EtOH aq.).

Di-Me ester:
$C_{14}H_{22}O_4$ M 254.3 Syrup. d_4^{20} 1.0706. Bp_{11} 159-167°. n_D^{20} 1.4730.

Dinitrile: [85688-88-6]. *1,1′-Dicyano-1,1′-bicyclopentyl*
$C_{12}H_{16}N_2$ M 188.2 Cryst. (petrol or Et_2O). Mp 98.5-99° (94-96°).

Overberger, C.G. *et al*, *J.A.C.S.*, 1951, **73**, 4883 (*dinitrile*)
Overberger, C.G. *et al*, *J.O.C.*, 1955, **20**, 1717 (*synth*)
Eberson, L., *Acta Chem. Scand.*, 1959, **13**, 40, 211 (*pKa*)
Tan, B.G. *et al*, *J.C.S. Perkin 2*, 1990, 2031; 1991, 937 (*dinitrile, ir, Raman*)
Kohl, L.L. *et al*, *Acta Cryst. C*, 1992, **48**, 1641 (*cryst struct, dinitrile*)

Bicyclo[4.4.1]undecan-11-one B-1-00100



$C_{11}H_{18}O$ M 166.2

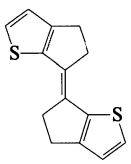
(1RS,6RS)-form
trans-*form*
Strained 'inside-outside' bicyclo system. Model for ingenane diterpenes. No phys. props. reported.

Winkler, J.D. *et al*, *J.A.C.S.*, 1994, **116**, 4183 (*synth, pmr, cmr*)

6,6′-Bi(4,5-dihydro-6*H*-cyclopenta[*b*]thienylidene) B-1-00101

*6-(4,5-Dihydro-6*H*-cyclopenta*[b]*thien-6-ylidene)-5,6-dihydro-4*H*-cyclopenta*[b]*thiophene, 9CI*

[158962-72-2]



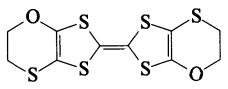
$C_{14}H_{12}S_2$ M 244.3

(E)-form
Orange powder. Mp 205°.

Roncali, J. *et al*, *Chem. Comm.*, 1994, 2249 (*synth, pmr*)

2,2′-Bi(5,6-dihydro-1,3-dithiolo[4,5-*b*][1,4]oxathiin-2-ylidene) B-1-00102

*2-(5,6-Dihydro-1,3-dithiolo[4,5-*b*][1,4]oxathiin-2-ylidene)-5,6-dihydro-1,3-dithiolo[4,5-*b*][1,4]oxathiin, 9CI. Bis(dihydro-1,4-oxathiino) tetrathiafulvalene*



(*E*)-*form*

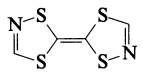
$C_{10}H_8O_2S_6$ M 352.5
Donor for cation radical salts. Obt. as mixt. of (*E*)- and (*Z*)-isomers which could not be separated.

[156119-21-0, 156119-24-3]

Hellberg, J. *et al*, *Chem. Comm.*, 1994, 817 (*synth, pmr, cmr, ms, use*)

5,5′-Bi(1,4,2-dithiazol-5-ylidene) B-1-00103

5-(1,4,2-Dithiazol-5-ylidene)-1,4,2-dithiazole, 9CI



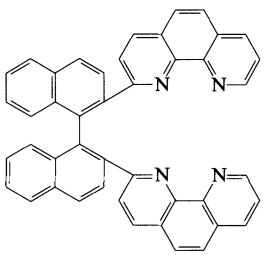
(*E*)-*form*

$C_4H_2N_2S_4$ M 206.3
Obt. as mixt. of *E* and *Z-forms*. Electron donor. Red solid.

[155934-53-5, 155934-54-6]

Oakley, R.T. *et al*, *J.O.C.*, 1994, **59**, 2997 (*synth, cryst struct, uv, pmr, cmr, ms*)

2,2′-[1,1′-Binaphthalene]-2,2′-diylbis-1,10-phenanthroline, 9CI B-1-00104



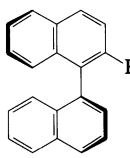
$C_{44}H_{26}N_4$ M 610.7
Helically chiral ligand.

(±)-***form*** [155351-45-4]
Cryst. as dihydrate (MeOH). Mp 360-362° dec.

Judice, J.K. *et al*, *Chem. Comm.*, 1993, 1323 (*synth*)

[1,1′-Binaphthalen-2-yl]diphenylphosphine B-1-00105

2-(Diphenylphosphino)-1,1′-binaphthalene



(*S*)-*form*

$C_{32}H_{23}P$ M 438.5

(S)-form [156456-77-8]
$[\alpha]_D^{20}$ +102.4 (c, 2.03 in $CHCl_3$).

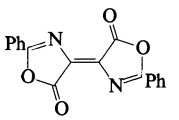
P-*Oxide:* [132532-07-1].
$C_{32}H_{23}OP$ M 454.5 $[\alpha]_D^{20}$ +15.5 (c, 0.77 in CH_2Cl_2).

Uozumi, Y. *et al*, *Tetrahedron*, 1994, **50**, 4293 (*synth, pmr, P-31 nmr*)

Δ$^{4,4'}$-Bi(5-oxo-2-phenyl-4(5*H*)-oxazole) B-1-00106

*4-(5-Oxo-2-phenyl-4(5*H*)-oxazolylidene)-2-phenyl-5(4*H*)-oxazolone, 9CI. Hippurorubrine*

[72884-72-1]

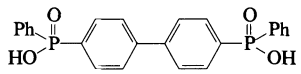


$C_{18}H_{10}N_2O_4$ M 318.2

(±)-***form***
Obt. from *N*-Benzoylglycine, B-0-01282. Red cryst. (diphenyl ether). Mp 305-308° dec.

Stachel, H.-D. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1979, **312**, 968 (*synth, cryst struct, uv, ir*)

[1,1′-Biphenyl]-4,4′-diyl(phenylphosphinic acid) B-1-00107

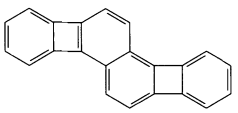


$C_{24}H_{20}O_4P_2$ M 434.3
Solid. Mp 213-215°.

Baldwin, R.A. *et al*, *J.O.C.*, 1967, **32**, 1572.

Biphenyleno[2,1-*a*]biphenylene B-1-00108

[157722-35-5]

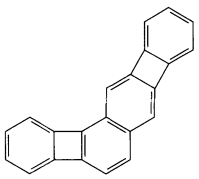


$C_{22}H_{12}$ M 276.3
Deep red cryst. Mp >200°. Part. dec. >150°.

Shepherd, M.K., *J.C.S. Perkin 1*, 1994, 1055 (*synth, pmr*)

Biphenyleno[2,3-*a*]biphenylene, 9CI B-1-00109

[107369-34-6]

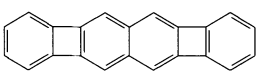


$C_{22}H_{12}$ M 276.3
Deep yellow cryst. (hexane). Mp 187-189°.

Barton, J.W. *et al*, *J.C.S. Perkin 1*, 1986, 967.

Biphenyleno[2,3-*b*]biphenylene, 9CI B-1-00110

[87837-26-1]

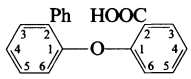


$C_{22}H_{12}$ M 276.3
Pale yellow leaflets. Mp >360°.

Helson, H.E. *et al, Angew. Chem., Int. Ed.*, 1985, **24**, 114 (*synth*)
Barton, J.W. *et al, J.C.S. Perkin 1*, 1986, 967 (*synth, pmr*)

2-(2-Biphenylyloxy)benzoic acid B-1-00111

2-(2-Phenylphenoxy)benzoic acid. 2'-Phenyldiphenyl ether-2-carboxylic acid



$C_{19}H_{14}O_3$ M 290.3
Needles (C_6H_6/hexane). Mp 156-157°.

Troshchenko, A.T., *Zh. Obshch. Khim.*, 1957, **27**, 967; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1957, **27**, 1047 (*synth*)

2-(4-Biphenylyloxy)benzoic acid B-1-00112

2-(4-Phenylphenoxy)benzoic acid. 4'-Phenyldiphenyl ether-2-carboxylic acid

$C_{19}H_{14}O_3$ M 290.3
Needles (C_6H_6/petrol). Mp 148-150°. Gives yellow colour in H_2SO_4.

Troshchenko, A.T., *Zh. Obshch. Khim.*, 1957, **27**, 967; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1957, **27**, 1047 (*synth*)
Mustafa, A. *et al, J.O.C.*, 1960, **25**, 1519 (*synth*)

4-(2-Biphenylyloxy)benzoic acid B-1-00113

4-(2-Phenylphenoxy)benzoic acid. 2'-Phenyldiphenyl ether-4-carboxylic acid

[125038-78-0]

$C_{19}H_{14}O_3$ M 290.3
Monomer for polyether ketones. Pale orange cryst. (EtOH aq.). Mp 160-161°.

Ueda, M. *et al, Polym. J. (Tokyo)*, 1989, **21**, 673 (*synth, ir*)

4-(4-Biphenylyloxy)benzoic acid B-1-00114

4-(4-Phenylphenoxy)benzoic acid. 4'-Phenyldiphenyl ether-4-carboxylic acid

[48193-94-8]

$C_{19}H_{14}O_3$ M 290.3
Cryst. (2-dichlorobenzene). Mp 243-244°.

Me ester: [48198-80-7].
$C_{20}H_{16}O_3$ M 304.3 Pseudoretinoid. Cryst. (hexane/Et_2O). Mp 158-160°.

Et ester: [48203-16-3].
$C_{21}H_{18}O_3$ M 318.3 Cryst. Mp 75.5-76.5°.

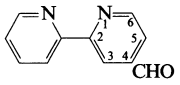
Chloride: [39033-48-2].
$C_{19}H_{13}ClO_2$ M 308.7 Cryst. Mp 93.5-94.5°.

U.S. Pat., 4 229 564, (1980); *CA*, **94**, 84840a (*synth, esters, chloride, ir*)
Sutherlin, D.M. *et al, Macromolecules*, 1985, **18**, 2669 (*Me ester*)
Torrado, A. *et al, Synthesis*, 1995, 285 (*Me ester*)

[2,2'-Bipyridine]-4-carboxaldehyde, 9CI B-1-00115

4-Formyl-2,2'-bipyridine

[146581-82-0]



$C_{11}H_8N_2O$ M 184.1
Solid. Mp 84.8-86.0°.

Imperiali, B. *et al, J.O.C.*, 1993, **58**, 1613 (*synth, pmr, cmr, ir, uv*)

[2,2'-Bipyridine]-6-carboxaldehyde, 9CI B-1-00116

6-Formyl-2,2'-bipyridine

[134296-07-4]

$C_{11}H_8N_2O$ M 184.1
Oil.

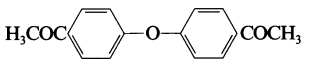
Phenylhydrazone: [134296-08-5].
Yellow solid (EtOH aq.). Mp 125-127°.

Goodwin, H.A. *et al, Aust. J. Chem.*, 1991, **44**, 331 (*synth, ir, pmr*)

Bis(4-acetylphenyl) ether B-1-00117

4',4'''-Oxydiacetophenone, 8CI. 4,4'-Diacetyldiphenyl ether

[2615-11-4]



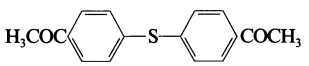
$C_{16}H_{14}O_3$ M 254.2
Mp 100-101°.

Royles, B.J.L. *et al, J.C.S. Perkin 1*, 1994, 355 (*synth*)

Bis(4-acetylphenyl) sulfide B-1-00118

4',4'''-Thiodiacetophenone, 8CI. 4,4'-Diacetyldiphenyl sulfide

[2615-09-0]



$C_{16}H_{14}O_2S$ M 270.3
Mp 90-91° (85-87°).

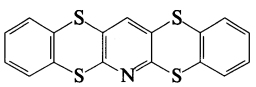
S,S-*Dioxide: Bis(4-acetylphenyl) sulfone*
$C_{16}H_{14}O_4S$ M 302.3 Cryst. (AcOH aq.). Mp 209°.

Royles, B.J.L. *et al, J.C.S. Perkin 1*, 1994, 355 (*synth, pmr*)

Bis[1,4]benzodithiino[2,3-*b*:2',3'-*e*]pyridine, 9CI B-1-00119

6-Aza-5,7,12,14-tetrathiapentacene

[158696-60-7]

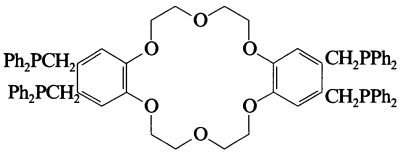


$C_{17}H_9NS_4$ M 355.5
Cryst. (toluene). Mp 247°.

Marti, C. *et al, J.O.C.*, 1994, **59**, 6200 (*synth, pmr, cmr, ms, cryst struct, epr*)

Bis[4,5-bis(diphenylphosphino) benzo]-18-crown-6 B-1-00120

[(*6,7,9,10,17,18,20,21-Octahydrodibenzo*[b,k][*1,4,7,10,13,16*] *hexaoxacyclooctadecin-2,3,13,14-tetrayl*)] *tetrakis(methylene)tetrakis[diphenylphosphine]*



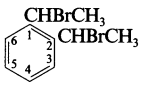
$C_{72}H_{68}O_6P_4$ M 1153.2

Tetraoxide: [88928-02-3].
$C_{72}H_{68}O_{10}P_4$ M 1217.2 Selectively extracts U(*VI*) and Pu(*IV*) from Am(*III*) in 3*M* HNO_3. Cryst. (EtOH/$CHCl_3$). Mp >325°.

Myasaedov, B.F. *et al, Solvent Extr. Ion Exch.*, 1983, **1**, 689 (*props, use*)
Bodrin, G.V. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1984, 1841; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1984, 1682 (*oxide, synth*)

1,2-Bis(1-bromoethyl)benzene B-1-00121

[58083-44-6]



$C_{10}H_{12}Br_2$ M 292.0
Prisms (CH_2Cl_2). Mp 91°. Mixt. of stereoisomers.

[147008-27-3, 147008-28-4]

Deluchat, R., *C. R. Hebd. Seances Acad. Sci.*, 1931, **192**, 1387 (*synth*)
Klimovitskii, E.N. *et al, Zh. Org. Khim.*, 1992, **28**, 253 (*synth, resoln*)
Eru, E. *et al, Tetrahedron*, 1995, **51**, 3033 (*synth, pmr*)

1,4-Bis(1-bromoethyl)benzene B-1-00122

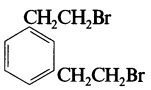
[17194-87-5]

$C_{10}H_{12}Br_2$ M 292.0
Cryst. (Et_2O). Mp 112°.

Ingle, H., *Ber.*, 1894, **27**, 2526 (*synth*)
Davy, J.R. *et al, Aust. J. Chem.*, 1979, **32**, 1067 (*synth*)

1,3-Bis(2-bromoethyl)benzene B-1-00123

[103199-07-1]



$C_{10}H_{11}Br_2$ M 291.0
Oil. $Bp_{0.05}$ 110-119°.

Ruggli, P. *et al, Helv. Chim. Acta*, 1945, **28**, 674 (*synth*)

Bis(2-bromoethyl)selenide B-1-00124

1,1'-Selenobis[*2-bromoethane*], *9CI. 2,2'-Dibromodiethyl selenide*

[41294-57-9]

$BrCH_2CH_2SeCH_2CH_2Br$

$C_4H_8Br_2Se$ M 294.8

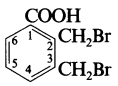
Yellow needles (EtOH). Mp 44.2°.

Dichloride:
$C_4H_8Br_2Cl_2Se$ M 365.7 Pale yellow prisms ($CHCl_3$). Mp 98-99°.

Dibromide: Dibromobis(2-bromoethyl)(T-4) selenium, 9CI
$C_4H_8Br_4Se$ M 454.6 Bright yellow prisms ($CHCl_3$). Mp 118°.

Bell, H.C. *et al, J.C.S.*, 1925, 1877 (*synth*)

2,3-Bis(bromomethyl)benzoic acid B-1-00125



$C_9H_8Br_2O_2$ M 307.9

Nitrile: [66126-18-9]. *1,2-Bis(bromomethyl)-3-cyanobenzene*
$C_9H_7Br_2N$ M 288.9 Cryst. (MeOH). Mp 93°.

Eru, E. *et al, Tetrahedron*, 1995, **51**, 3033 (*synth, pmr*)

2,4-Bis(bromomethyl)benzoic acid B-1-00126

$C_9H_8Br_2O_2$ M 307.9

Me ester: [63112-94-7].
$C_{10}H_{10}Br_2O_2$ M 321.9 Oil.

Newman, M.S. *et al, J.A.C.S.*, 1968, **90**, 4410 (*synth*)
Meyer, A. *et al, Chem. Ber.*, 1977, **110**, 1403 (*synth*)

2,5-Bis(bromomethyl)benzoic acid B-1-00127

[148692-70-0]

$C_9H_8Br_2O_2$ M 307.9

Me ester: [74725-06-7].
$C_{10}H_{10}Br_2O_2$ M 321.9 Cryst. (cyclohexane). Mp 83°.

Hibert, M. *et al, J.O.C.*, 1980, **45**, 4496 (*Me ester, synth, pmr*)
Benniston, A.C. *et al, Synlett*, 1993, 223 (*synth, ir, pmr*)

2,6-Bis(bromomethyl)benzoic acid B-1-00128

[56263-54-8]

$C_9H_8Br_2O_2$ M 307.9
Cryst. (Me_2CO). Mp 120° dec.

Me ester: [56263-51-5].
$C_{10}H_{10}Br_2O_2$ M 321.9 Cryst. (CH_2Cl_2/MeOH). Mp 74-76°.

Nitrile: [33875-63-7]. *1,3-Bis(bromomethyl)-2-cyanobenzene*
$C_9H_7Br_2N$ M 288.9 Cryst. ($CHCl_3$). Mp 98-101°.

Vögtle, F. *et al, Chem. Ber.*, 1972, **105**, 2955; 1975, **108**, 1694.

3,4-Bis(bromomethyl)benzoic acid B-1-00129

[20896-24-6]

$C_9H_8Br_2O_2$ M 307.9
Cryst. Mp 170-177°.

Me ester: [20896-23-5].
$C_{10}H_{10}Br_2O_2$ M 321.9 Cryst. (petrol). Mp 74.5-75°.

[66126-17-8]

Wynberg, H. *et al, Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1968, **87**, 1006 (*synth, Me ester, uv, ir, pmr*)
Rogers, G.A., *Anal. Biochem.*, 1977, **78**, 406.

3,5-Bis(bromomethyl)benzoic acid B-1-00130

[94111-75-8]

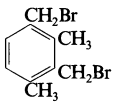
$C_9H_8Br_2O_2$ M 307.9
Cysteine crosslinking agent. Needles (EtOAc/hexane). Mp 161-163°.

Me ester: [29333-41-3].
$C_{10}H_{10}Br_2O_2$ M 321.9 Cryst. (Et_2O). Mp 100-101°.

Nitrile: [74163-48-7]. *1,3-Bis(bromomethyl)-5-cyanobenzene*
$C_9H_7Br_2N$ M 288.9 Cryst. (CCl_4/hexane). Mp not given.

Staab, H.A. *et al, Annalen*, 1979, 886 (*synth, Me ester, pmr*)
Engel, M. *et al, Tetrahedron*, 1993, **49**, 8761 (*synth, pmr*)
Karlin, K.D. *et al, J.A.C.S.*, 1994, **116**, 1324 (*synth, nitrile, pmr*)

1,3-Bis(bromomethyl)-2,4-dimethylbenzene B-1-00131



$C_{10}H_{12}Br_2$ M 292.0
Mp 69°.

Grimme, S. *et al, J.A.C.S.*, 1995, **117**, 157 (*synth, pmr, cmr, ms*)

2,5-Bis(bromomethyl)-1,3-dimethylbenzene B-1-00132

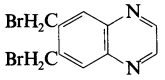
[148873-79-4]

$C_{10}H_{12}Br_2$ M 292.0
Cryst. (cyclohexane). Mp 140-142°.

Lai, Y.-H. *et al, J.C.S. Perkin 2*, 1993, 703 (*synth, ir, pmr, ms*)
Lai, Y.-H. *et al, J.O.C.*, 1994, **59**, 3381 (*synth*)

6,7-Bis(bromomethyl) quinoxaline, 9CI B-1-00133

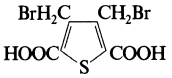
[143154-10-3]



$C_{10}H_8Br_2N_2$ M 315.9
Amber oil.

Baudy, R.B. *et al, J. Med. Chem.*, 1993, **36**, 331 (*synth, pmr*)

3,4-Bis(bromomethyl)-2,5-thiophenedicarboxylic acid B-1-00134



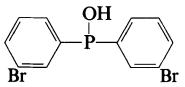
$C_8H_6Br_2O_4S$ M 358.0

Di-Me ester:
$C_{10}H_{10}Br_2O_4S$ M 386.0 Cryst. (MeOH/petrol). Mp 124.5-126°.

Dinitrile: [155632-48-7]. *3,4-Bis(bromomethyl)-2,5-dicyanothiophene*
$C_8H_4Br_2N_2S$ M 320.0 Cryst. (MeOH). Mp 127-129°.

Wynberg, H. *et al, J.O.C.*, 1964, **29**, 1919 (*Di-Me ester, synth, uv, pmr*)
Beye, N. *et al, J.O.C.*, 1994, **59**, 2223 (*dinitrile, synth, pmr, ir, uv, ms*)

Bis(3-bromophenyl) phosphinous acid, 9CI B-1-00135



$C_{12}H_9Br_2OP$ M 359.9
Tautomeric.

Et ester: [13685-48-8]. *Ethyl bis(3-bromophenyl)phosphinite*
$C_{14}H_{13}Br_2OP$ M 388.0 Liq. d_4^{20} 1.54. Bp_2 162-164°. n_D^{20} 1.6296.

Chloride: [13685-29-5]. *Bis(3-bromophenyl) chlorophosphine*
$C_{12}H_8Br_2ClP$ M 378.4 Liq. with strong odour. d_4^{20} 1.72. Bp_3 175-176°. n_D^{20} 1.6724.

Yudina, K.S. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1966, 1954; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1966, 1889 (*synth*)

Bis(4-bromophenyl) phosphinous acid B-1-00136

$C_{12}H_9Br_2OP$ M 359.9

Et ester: [13792-91-1]. *Ethyl bis(4-bromophenyl)phosphinite*
$C_{14}H_{13}Br_2OP$ M 388.0 Liq. d_4^{20} 1.51 (1.37). Bp_5 200-203°, Bp_2 154-156°. n_D^{20} 1.6261.

Propyl ester: [23055-23-4]. *Propyl bis(4-bromophenyl)phosphinite*
$C_{15}H_{15}Br_2OP$ M 402.0 Liq. d_4^{20} 1.47. Bp_5 205-207°. n_D^{20} 1.6142.

Ph ester: [65924-33-6]. *Phenyl bis(4-bromophenyl)phosphinite*
$C_{18}H_{13}Br_2OP$ M 436.0 $Bp_{0.6}$ 210-214°. n_D^{20} 1.6600.

Chloride: [13685-28-4]. *Bis(4-bromophenyl) chlorophosphine*
$C_{12}H_8Br_2ClP$ M 378.4 Solid. Mp 72-75°. Bp_3 177-179°.

Yudina, K.S. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1966, 1954; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1966, 1889 (*chloride, ester*)
Kamai, G. *et al, Zh. Obshch. Khim.*, 1969, **39**, 625; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1969, **39**, 592 (*Et ester, chloride*)
Kharrasova, F.M. *et al, Zh. Obshch. Khim.*, 1978, **48**, 1046; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1978, **48**, 953 (*Ph ester, synth, P-31 nmr*)

Bis(carboxymethyl)phosphinic acid B-1-00137

2,2′-Phosphinicobisacetic acid

[134150-73-5]

$(HOOCCH_2)_2P(O)OH$

$C_4H_7O_6P$ M 182.0
Solid. Mp 108-110°.

Di-Me ester: [126443-46-7]. *1,1'-Dimethyl 2,2'-phosphinicobisacetate*
$C_6H_{11}O_6P$ M 210.1 Solid. Mp 63-64°.

C-*Di-Me ester*, P-*trimethylsilyl ester:*
$C_9H_{19}O_6PSi$ M 282.3 Liq. $Bp_{0.6}$ 110°.

Majewski, P., *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1989, **45**, 151 (*ester, synth, ir, pmr, P-31 nmr*)
Bondarenko, N.A. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **56**, 179 (*synth, P-31 nmr*)

Bis(2-chloroethyl) selenide B-1-00138

1,1'-Selenobis[2-chloroethane]

$ClCH_2CH_2SeCH_2CH_2Cl$

$C_4H_8Cl_2Se$ M 205.9
Needles. Mp 24.2°. Unstable.

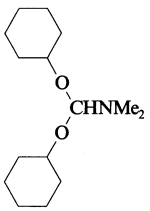
Se,Se-*Dichloride:*
$C_4H_8Cl_4Se$ M 276.8 Long prisms ($CHCl_3$). Mp 122.5°.

Se,Se-*Dibromide:*
$C_4H_8Br_2Cl_2Se$ M 365.7 Pale yellow prisms ($CHCl_3$). Mp 117° dec.

Bausor, H.W. *et al*, *J.C.S.*, 1920, **117**, 1453 (*dichloride*)
Bell, H.C. *et al*, *J.C.S.*, 1925, **27**, 1877 (*synth*)

1,1-Bis(cyclohexyloxy) trimethylamine, 8CI B-1-00139

1,1-Bis(cyclohexyloxy)-N,N-dimethylmethanamine, 9CI.
Dimethylformamide dicyclohexyl acetal
[2016-05-9]

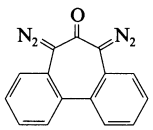


$C_{15}H_{29}NO_2$ M 255.4
Dye intermed. d 0.96. $Bp_{0.75}$ 115-116°. n_D^{25} 1.4685.

Arnold, Z. *et al*, *Coll. Czech. Chem. Comm.*, 1964, **29**, 645.
Swiss Pat., 384 564, (1965); *CA*, **62**, 16135h (*manuf*)

5,7-Bis(diazo)-5,7-dihydro-6*H*-dibenzo[*a*,*c*]cyclohepten-6-one, 9CI B-1-00140

[166042-86-0]



$C_{15}H_8N_4O$ M 260.2
Orange solid. Mp 164-165° dec.

Tomioka, H. *et al*, *J.O.C.*, 1995, **60**, 2344 (*synth, pmr, ir*)

2,6-Bis(dibromomethyl) benzoic acid, 9CI B-1-00141

[14346-75-9]

$C_9H_6Br_4O_2$ M 465.7
Mp 203-206°.

Francis, J.E. *et al*, *Can. J. Chem.*, 1979, **57**, 3320 (*synth*)

3,4-Bis(dibromomethyl) benzoic acid, 9CI B-1-00142

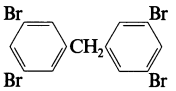
[19047-21-3]

$C_9H_6Br_4O_2$ M 465.7
Cryst. ($CHCl_3$/Me_2CO). Mp 224-226°.

Amano, T. *et al*, *Yakugaku Zasshi*, 1968, **88**, 247; *CA*, **69**, 59029u (*synth, pmr*)
Kleisch, H. *et al*, *Annalen*, 1995, 1269 (*synth, ir, pmr, ms*)

Bis(3,5-dibromophenyl) methane B-1-00143

1,1'-Methylenebis[3,5-dibromobenzene], 9CI.
3,3',5,5'-Tetrabromodiphenylmethane
[160976-67-0]



$C_{13}H_8Br_4$ M 483.8
Cryst. Mp 192-193°.

Rajca, A. *et al*, *J.O.C.*, 1994, **59**, 7701 (*synth, ms, pmr, cmr, ir*)

Bis[(di-*tert*-butylphosphino) methyl]methylphosphine B-1-00144

Bis[[bis(1,1-dimethylethyl)phosphino]methyl] methylphosphine, 9CI
[153995-47-2]

$[(H_3C)_3C]_2PCH_2PMeCH_2P[C(CH_3)_3]_2$

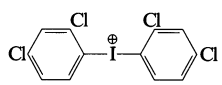
$C_{19}H_{43}P_3$ M 364.4
Solid. Mp 112°.

Trisulfide: [153995-48-3]. *Bis[[bis(1,1-dimethylethyl)phosphinothioyl]methyl] methylphosphine sulfide*
$C_{19}H_{43}P_3S_3$ M 460.6 Cryst. (Et_2O).

Krill, J. *et al*, *Chem. Ber.*, 1993, **126**, 2379 (*synth, ms, pmr, cmr, P-31 nmr*)

Bis(2,4-dichlorophenyl) iodonium(1+), 9CI B-1-00145

Feniodium(1+)
[71585-34-7]



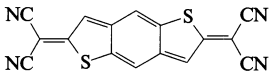
$C_{12}H_6Cl_4I^{\oplus}$ M 418.8 (ion)

Chloride: [34563-73-0]. ***Feniodium chloride, INN. Chlodophen***
$C_{12}H_6Cl_5I$ M 454.3 Anthelmintic.
▶ LD_{Lo} (mus, ipr) 250 mg/kg. NN6300000.
[34106-48-4]

Pershin, G.N. *et al*, *CA*, 1971, **75**, 61988 (*pharmacol*)
Nilsson, C.-A. *et al*, *Chemosphere*, 1977, **6**, 599 (*synth*)

2,6-Bis(dicyanomethylene)-2,6-dihydrobenzo[1,2-*b*:4,5-*b'*]dithiophene B-1-00146

2,2'-Benzo[1,2-b:4,5-b']dithiophene-2,6-diylidenebispropanedinitrile, 9CI
[153288-76-7]

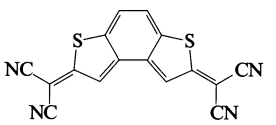


$C_{16}H_4N_4S_2$ M 316.3
Electron acceptor, forms electrically conductive charge-transfer complexes with electron donors. Deep violet fine cryst. (CH_2Cl_2). Mp >300°.

Yoshida, S. *et al*, *J.O.C.*, 1994, **59**, 3077 (*synth, uv, ir, use*)

2,7-Bis(dicyanomethylene)-2,7-dihydrobenzo[1,2-*b*:4,3-*b'*]dithiophene B-1-00147

2,2'-Benzo[1,2-b:4,3-b']dithiophene-2,7-diylidenebispropanedinitrile, 9CI
[156355-42-9]

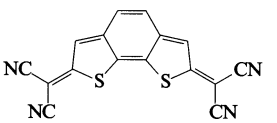


$C_{16}H_4N_4S_2$ M 316.3
Electron acceptor, forms electrically conductive charge-transfer complexes. Fine green cryst. Mp >300° dec. Solns. are air sensitive.

Yoshida, S. *et al*, *J.O.C.*, 1994, **59**, 3077 (*synth, uv, ir, use*)

2,7-Bis(dicyanomethylene)-2,7-dihydrobenzo[2,1-*b*:3,4-*b'*]dithiophene B-1-00148

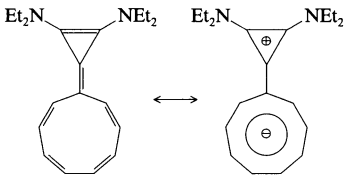
2,2'-Benzo[2,1-b:3,4-b']dithiophene-2,7-diylidenebispropanedinitrile, 9CI
[156355-41-8]



$C_{16}H_4N_4S_2$ M 316.3
Electron acceptor, forms conducting charge-transfer complexes with many common electron donors. Bluish-violet fine cryst. (PhCl). Mp 226° dec.

Yoshida, S. *et al*, *J.O.C.*, 1994, **59**, 3077 (*synth, uv, ir, pmr, use*)

11,12-Bis(diethylamino) nonatriafulvalene B-1-00149



$C_{20}H_{28}N_2$ M 296.4

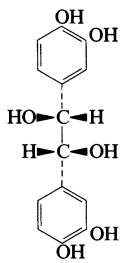
'Aromatic' nonafulvene showing delocalisation to a dipolar struct. Pale yellow cubes (CH_2Cl_2/Et_2O at −70°). Stable for several days at r.t. under Ar, polymerises rapidly in air.

Chai, S. *et al*, *Angew. Chem., Int. Ed.*, 1994, **33**, 973 (*synth, ir, uv, pmr, cmr*)

1,2-Bis(3,4-dihydroxyphenyl)-1,2-ethanediol B-1-00150

4,4′-(1,2-Dihydroxy-1,2-ethanediyl)bis-1,2-benzenediol, 9CI

[74240-25-8]



(*1R*,2R**)-*form*

$C_{14}H_{14}O_6$ M 278.2

(1R*,2R*)-form

3′,3″,4′,4″-Tetra-Me ether: 1,2-Bis(3,4-dimethoxyphenyl)-1,2-ethanediol. Hydroveratroin
$C_{18}H_{22}O_6$ M 334.3 $[\alpha]_D$ +135 (c, 3 in Me_2CO).

(1S*,2S*)-form

3′,3″,4′,4″-Tetra-Me ether: $[\alpha]_D$ −135 (c, 3 in Me_2CO).

(1RS,2RS)-form

(±)-*form*

3′,3″,4′,4″-Tetra-Me ether: Mp 150-170° (dehydrates). Crystallises as a conglomerate showing spontaneous resolution.

(1RS,2SR)-form

meso-*form*

3′,3″-Di-Me ether: 1,2-Bis(4-hydroxy-3-methoxyphenyl)-1,2-ethanediol. meso-*Hydrovanilloin*
$C_{16}H_{18}O_6$ M 306.3 Mp 229-232°.

3′,3″,4′,4″-Tetra-Me ether: Cryst. Mp 210-211°.

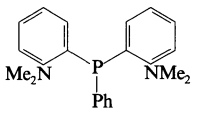
Grimshaw, J. *et al*, *J.C.S.(C)*, 1966, 653 (*synth, bibl*)

Karlsson, O. *et al*, *Acta Chem. Scand.*, 1993, **47**, 728 (*synth, cryst struct, tetra-Me ether*)

Bis[2-(dimethylamino)phenyl] phenylphosphine B-1-00151

2,2′-(Phenylphosphinidene)bis[N,N-*dimethylbenzenamine*]

[4551-07-9]



$C_{22}H_{25}N_2P$ M 348.4

Ligand for Pd, Pt and Ir. Complexes used in chemoselective and enantioselective hydrogenations. Cryst. (EtOH aq.). Mp 95° (82-85°).

Phenylmethobromide:
$C_{29}H_{32}BrN_2P$ M 519.4 Solid. Mp 254-257°.

Fritz, H.P. *et al*, *J.C.S.*, 1965, 5210 (*synth, complexes*)

Horner, L. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1983, **15**, 165 (*synth*)

Cairns, S.M. *et al*, *Heteroat. Chem.*, 1990, **1**, 9 (*synth, deriv, uv, ir, pmr, cmr, P-31 nmr*)

Mashima, K. *et al*, *J. Organomet. Chem.*, 1992, **428**, 213 (*complex, use*)

Zhang, X. *et al*, *J.A.C.S.*, 1993, **115**, 3318 (*complex, use*)

Zhang, X. *et al*, *Tetrahedron: Asymmetry*, 1994, **5**, 1179 (*complex, use*)

Bis[3-(dimethylamino)phenyl] phenylphosphine B-1-00152

3,3′-(Phenylphosphinidene)bis[N,N-*dimethylbenzenamine*], *9CI*

[79462-60-5]

$C_{22}H_{25}N_2P$ M 348.4

P-*Oxide:* [131981-42-5]. *3,3′-(Phenylphosphinylidene)bis*[N,N-*dimethylbenzenamine*]
$C_{22}H_{25}N_2OP$ M 364.4 Cryst. (Me_2CO). Mp 169-171°.

Pervukhina, I.N. *et al*, *Zh. Obshch. Khim.*, 1990, **60**, 1558; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1990, **60**, 1392 (*synth, cmr*)

Bis[4-(dimethylamino)phenyl] phenylphosphine B-1-00153

4,4′-(Phenylphosphinidene)bis[N,N-*dimethylbenzenamine*]

[1100-11-4]

$C_{22}H_{25}N_2P$ M 348.4

Ligand for Au. Cryst. (EtOH). Mp 151°.

Methiodide:
$C_{23}H_{28}IN_2P$ M 490.3 Cryst. (H_2O). Mp 160-168°.

Phenylmethobromide:
$C_{29}H_{32}BrN_2P$ M 519.4 Solid. Mp 270°.

P-*Oxide: 4,4′-(Phenylphosphinylidene) bis*[N,N-*dimethylbenzenamine*]
$C_{22}H_{25}N_2OP$ M 364.4 Cryst. (MeOH aq.). Mp 203.5-204.5°.

P-*Sulfide:* [1100-95-4]. *4,4′-(Phenylphosphinothioylidene)bis*[N,N-*dimethylbenzenamine*]
$C_{22}H_{25}N_2PS$ M 380.4 Cryst. (C_6H_6). Mp 219-220°.

Schiemenz, G.P., *Chem. Ber.*, 1965, **98**, 65 (*synth, derivs*)

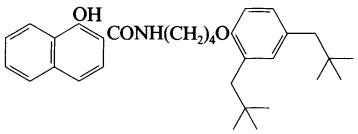
Horner, L. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1983, **15**, 165 (*synth*)

Cairns, S.M. *et al*, *Heteroat. Chem.*, 1990, **1**, 9 (*synth, derivs, uv, ir, pmr, cmr, P-31 nmr*)

Schmidbaur, H. *et al*, *Z. Naturforsch., B*, 1992, **47**, 1725 (*complexes*)

N-[4-[2,4-Bis(1,1-dimethylpropyl)phenoxy] butyl]-1-hydroxy-2-naphthalenecarboxamide, 9CI B-1-00154

[32180-75-9]



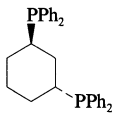
$C_{31}H_{41}NO_3$ M 475.6

Colour photographic complex, reacting with oxidised colour developer to yield cyan indoaniline image dyes.

Texter, J., *J. Photogr. Sci.*, 1988, **36**, 14.

Luss, H.R. *et al*, *Acta Cryst. C*, 1991, **47**, 1491 (*cryst struct*)

1,3-Bis(diphenylphosphino) cyclohexane B-1-00155



$C_{30}H_{30}P_2$ M 452.5

(1RS,3RS)-form

(±)-trans-*form*

Dioxide: [141874-91-1].
$C_{30}H_{30}O_2P_2$ M 484.5 Solid. Mp 282-283°.

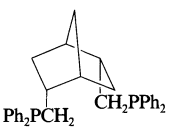
Morooka, M. *et al*, *Acta Cryst. C*, 1992, **48**, 1710 (*cryst struct*)

Hashimoto, T. *et al*, *Synlett*, 1992, 340 (*synth, ir*)

2,5-Bis[(diphenylphosphino) methyl]bicyclo[2.2.1]heptane B-1-00156

[*Bicyclo*[*2.2.1*]*heptane-2,5-diylbis*(*methylene*)] *bis*[*diphenylphosphine*], *9CI*

[76122-56-0]



$C_{33}H_{34}P_2$ M 492.5

(1RS,2RS,5RS)-form [80924-15-9]

(±)-endo,endo-*form*

Viscous liq.

[72151-44-1, 125282-09-9, 133362-45-5]

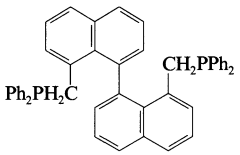
Casey, C.P. *et al*, *J.O.C.*, 1990, **55**, 1394 (*synth, pmr, cmr, P-31 nmr*)

Miyazawa, M. *et al*, *Synlett*, 1990, **11**, 711 (*synth*)

8,8′-Bis[(diphenylphosphino)methyl]-1,1′-binaphthalene B-1-00157

[[*1,1′-Binaphthalene*]-*8,8′-diylbis(methylene)*] *bis*[*diphenylphosphine*], *9CI*

[147151-95-9]



$C_{46}H_{36}P_2$ M 650.7
Solid. Mp 167-171°. Does not complex with Ni(*II*) or Pd(*II*).

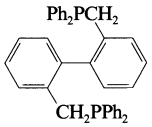
Dioxide:
$C_{46}H_{36}O_2P_2$ M 682.7 Solid. Mp 241-243°.

Widhalm, M. *et al*, *Monatsh. Chem.*, 1993, **124**, 103 (*synth*, *oxide*, *ms*, *pmr*, *P-31 nmr*, *cryst struct*)

2,2′-Bis[(diphenylphosphino)methyl]biphenyl B-1-00158

[[*1,1′-Biphenyl*]-*2,2′-diylbis(methylene)*] *bis*[*diphenylphosphine*], *9CI*

[111982-81-1]



$C_{38}H_{32}P_2$ M 550.6
Ligand for Mo and Rh. Complexes used in hydroformylation reaction.

[136379-28-7]

Herrmann, W.A. *et al*, *Inorg. Chem.*, 1991, **30**, 4271 (*synth*, *ir*, *ms*, *pmr*, *cmr*, *P-31 nmr*, *complexes*, *cryst struct*)
Casey, C.P. *et al*, *J.A.C.S.*, 1992, **114**, 5535, 10680 (*complexes*, *use*)

1,1-Bis[(diphenylphosphino)methyl]ethene B-1-00159

(*2-Methylene-1,3-propanediyl*) *bis*(*diphenylphosphine*)

[120658-80-2]

$(Ph_2PCH_2)_2C{=}CH_2$

$C_{28}H_{26}P_2$ M 424.4
Ligand for Pt. Cryst. (Me_2CO/MeOH). Mp 79-80°. Converted into carbanion by Me_3SiCH_2K.

Bismethiodide: [120883-37-6]. (*2-Methylene-1,3-propanediyl*) *bis*(*methyldiphenylphosphonium*)*diiodide*
$C_{30}H_{32}I_2P_2$ M 708.3 Solid. Mp 175-176°.

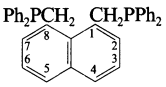
Disulfide: [120883-36-5].
$C_{28}H_{26}P_2S_2$ M 488.5 Cryst. (Me_2CO/MeOH). Mp 125°.

Schmidbaur, H. *et al*, *Chem. Ber.*, 1989, **122**, 1851 (*synth*, *ir*, *ms*, *pmr*, *cmr*, *P-31 nmr*)
van Doorn, J.A. *et al*, *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1990, **109**, 302 (*carbanion*)
Shaw, B.L. *et al*, *J.C.S. Dalton*, 1992, 1929 (*complexes*)

1,8-Bis[(diphenylphosphino)methyl]naphthalene B-1-00160

1,8-Naphthalenebis(methylene) *bis*(*diphenylphosphine*)

[73892-41-8]



$C_{36}H_{30}P_2$ M 524.5

Dioxide: [88928-06-7]. *1,8-Bis*[(*diphenylphosphinyl*)*methyl*]*naphthalene*
$C_{36}H_{30}O_2P_2$ M 556.5 Cryst. ($CHCl_3$). Mp 356-357°. Poor extractant for transuranic elements.

Myasoedov, B.F. *et al*, *Solvent Extr. Ion Exch.*, 1983, **1**, 689 (*use*)
Bodrin, G.V. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1984, 1841; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1984, 1682.
Kasachnik, M.I., *Heteroat. Chem.*, 1991, **2**, 1 (*props*, *use*)

2,3-Bis[(diphenylphosphino)methyl]naphthalene B-1-00161

2,3-Naphthalenediylbis(methylene) *bis*(*diphenylphosphine*)

$C_{36}H_{30}P_2$ M 524.5

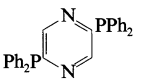
Dioxide: [88928-01-2]. *2,3-Bis*[(*diphenylphosphinyl*)*methyl*]*naphthalene*
$C_{36}H_{30}O_2P_2$ M 556.5 Selectively extracts U(*VI*) from Am(*III*), and Pu(*IV*) from Am(*III*) from acid soln. Cryst. (EtOH). Mp 286-287°.

Myasoedov, B.F. *et al*, *Solvent Extr. Ion Exch.*, 1983, **1**, 689 (*use*)
Bodrin, G.V. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1984, 1841; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1984, 1682 (*dioxide*, *synth*)
Kasachnik, M.I., *Heteroat. Chem.*, 1991, **2**, 1 (*props*)

2,5-Bis(diphenylphosphino)pyridazine B-1-00162

2,5-Pyridiazinediylbis(*diphenylphosphine*), *9CI*

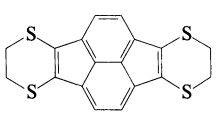
[127322-11-6]



$C_{28}H_{22}N_2P_2$ M 448.4
Ligand for Mo, W and Cr. Pale yellow cryst. (Me_2CO/MeOH). Mp 129-130°.

Zhang, Z.-Z. *et al*, *J. Organomet. Chem.*, 1990, **381**, 45 (*synth*, *P-31 nmr*, *complexes*, *cryst struct*)

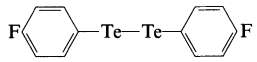
1,2:5,6-Bis(ethylenedithio)pyracyclene B-1-00163



$C_{18}H_{12}S_4$ M 356.5
Electron donor. Reversible two-stage redox compd. Mp 199-201°. No colour mentioned.

Tani, H., *Bull. Chem. Soc. Jpn.*, 1995, **68**, 661 (*synth*, *uv*, *cmr*, *ms*, *cryst struct*)

Bis(4-fluorophenyl)ditelluride B-1-00164



$C_{12}H_8F_2Te_2$ M 445.3
Dark red cryst. Mp 66-67°.

Crich, D. *et al*, *J.A.C.S.*, 1994, **116**, 8937 (*synth*, *pmr*)

Bis(4-fluorophenyl)ethanedione, 9CI B-1-00165

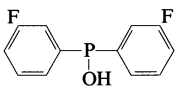
4,4′-Difluorobenzil

[579-39-5]

$C_{14}H_8F_2O_2$ M 246.2
Yellow needles (MeOH). Mp 120-122°.

Beak, P. *et al*, *J.O.C.*, 1976, **41**, 3389 (*synth*, *ir*, *pmr*, *ms*)
Bulman Page, P.C. *et al*, *Tetrahedron*, 1992, **48**, 7265 (*synth*, *ir*, *pmr*)

Bis(3-fluorophenyl)phosphinous acid B-1-00166



$C_{12}H_9F_2OP$ M 238.1
Free acid exists in tautomeric phosphoryl form.

Me ester: [23587-33-9]. *Methyl bis(3-fluorophenyl)phosphinite*
$C_{13}H_{11}F_2OP$ M 252.2 Liq. Bp_9 150°. n_D^{20} 1.5650.

Schindlbauer, H. *et al*, *Chem. Ber.*, 1969, **102**, 2914 (*methyl ester*, *synth*, *F-19 nmr*)
Kapoor, P.N. *et al*, *J. Organomet. Chem.*, 1984, **276**, 167 (*synth*)

Bis(4-fluorophenyl)phosphinous acid, 9CI B-1-00167

$C_{12}H_9F_2OP$ M 238.1

Me ester: [25186-20-3]. *Methyl bis(4-fluorophenyl)phosphinite*
$C_{13}H_{11}F_2OP$ M 252.2 Liq. Bp_{11} 145-148°. n_D^{20} 1.5619.

Chloride: [23039-97-6]. *Chlorobis(4-fluorophenyl)phosphine*
$C_{12}H_8ClF_2P$ M 256.6 Pungent liq. $Bp_{0.04}$ 108-110°. n_D^{20} 1.5890. Forms 1:1 adducts with BBr_3 and BCl_3.

Diethylamide: [25186-18-9]. N,N-*Diethyl*-P,P-*bis(4-fluorophenyl)phosphinous amide*. *Bis(4-fluorophenyl)phosphinous diethylamide*
$C_{16}H_{18}F_2NP$ M 293.2 Liq. Bp_{11} 172-175°, $Bp_{0.01}$ 110-113°. n_D^{20} 1.5620.

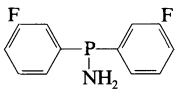
Dipropylamide: [25186-16-7]. P,P-*Bis(4-fluorophenyl)*-N,N-*dipropylphosphinous diamide*. *Bis(4-fluorophenyl)phosphinous dipropylamide*
$C_{18}H_{22}F_2NP$ M 321.3 Liq. Bp_{15} 198-199°. n_D^{20} 1.5486.

[57178-48-0, 57178-58-2]

De Ketelaere, R. *et al*, *Bull. Soc. Chim. Belg.*, 1969, **78**, 219 (*chloride*, *synth*, *ir*, *pmr*, *F-19 nmr*, *P-31 nmr*)
Prikoszovich, W. *et al*, *Chem. Ber.*, 1969, **102**, 2922.

Muylle, E. *et al, Spectrochim. Acta A*, 1975, **31**, 1039, 1045; 1976, **32**, 599 (*F-19 nmr, P-31 nmr*)

P,P-Bis(3-fluorophenyl) phosphinous amide, 9CI B-1-00168



$C_{12}H_{10}F_2NP$ M 237.1

N,N-*Di-Et:* [23588-25-2]. N,N-*Diethyl*-P,P-*bis(3-fluorophenyl)phosphinous amide. Bis(3-fluorophenyl)phosphinous diethylamide*
$C_{16}H_{18}F_2NP$ M 293.2 Liq. Bp_{12} 183°. n_D^{20} 1.5679.

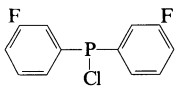
N,N-*Dipropyl:* [23588-18-3]. P,P-*Bis(3-fluorophenyl)*-N,N-*dipropylphosphinous amide. Bis(3-fluorophenyl)phosphonous dipropylamide*
$C_{18}H_{22}F_2NP$ M 321.3 Liq. Bp_{31} 217°. n_D^{20} 1.5511.

Schindlbauer, H. *et al, Chem. Ber.*, 1969, **102**, 2914.

Bis(3-fluorophenyl) phosphinous chloride, 9CI, 8CI B-1-00169

Chlorobis(3-fluorophenyl)phosphine

[23039-98-7]



$C_{12}H_8ClF_2P$ M 256.6

Liq. Bp_{22} 174°, Bp_1 116.5°. n_D^{20} 1.5934. Forms 1:1 complexes with BCl_3, BBr_3.

[57178-67-3, 57178-70-8]

De Ketelaare, R. *et al, Bull. Soc. Chim. Belg.*, 1969, **78**, 219 (*synth, ir, pmr, F-19 nmr, P-31 nmr*)

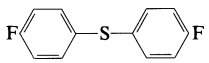
Schindlbaur, H. *et al, Chem. Ber.*, 1969, **102**, 2914 (*synth*)

Muylle, E. *et al, Spectrochim. Acta A*, 1975, **31**, 1039, 1045; 1976, **32**, 599 (*F-19 nmr, P-31 nmr, complexes*)

Bis(4-fluorophenyl)sulfide B-1-00170

1,1-Thiobis(4-fluorobenzene), 9CI. 4,4'-Difluorodiphenyl sulfide. Di(4-fluorophenyl) sulfide

[404-38-6]



$C_{12}H_8F_2S$ M 222.2

Mp 87-88°. Bp_9 136-137°.

S-*Oxide:* [395-25-5]. *1,1-Sulfinylbis[4-fluorobenzene], 9CI. Bis(4-fluorophenyl) sulfoxide*
$C_{12}H_8F_2OS$ M 238.2 Mp 51-52°.

S,S-*Dioxide:* [383-29-9]. *1,1-Sulfonylbis[4-fluorobenzene], 9CI. Bis(4-fluorophenyl) sulfone*
$C_{12}H_8F_2O_2S$ M 254.2 Mp 99-101°.

Jilek, J. *et al, Coll. Czech. Chem. Comm.*, 1984, **49**, 603 (*synth*)

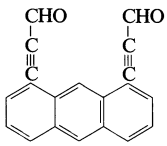
Chandrasekaran, R. *et al, Magn. Reson. Chem.*, 1987, **25**, 1001; 1989, **27**, 360 (*synth, pmr, cmr*)

Laali, K.K. *et al, J.O.C.*, 1991, **56**, 1867 (*synth, sulfoxide*)

1,8-Bis(2-formylethynyl) anthracene B-1-00171

3,3'-(1,8-Anthracendiyl)bis-2-propynal

[157993-36-7]



$C_{20}H_{10}O_2$ M 282.2

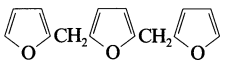
Yellow needles. Mp >250°.

Breitmaier, E. *et al, Annalen*, 1994, 857 (*synth, pmr, cmr, ms*)

2,5-Bis(2-furanylmethyl)furan B-1-00172

2,5-Difurfurylfuran

[29953-18-2]

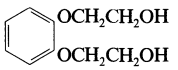


$C_{14}H_{12}O_3$ M 228.2

Bp_{1-2} 95-100°. Higher homologues having up to 7 furan rings also obt.

Musau, R.M. *et al, J.C.S. Perkin 1*, 1994, 2881 (*synth, uv, pmr, cmr*)

1,2-Bis(2-hydroxyethoxy) benzene B-1-00173



$C_{10}H_{14}O_4$ M 198.2

Cryst. (EtOH). Mp 74°.

Lüning, U. *et al, Chem. Ber.*, 1994, **127**, 2297.

1,2-Bis(hydroxymethoxy) ethane B-1-00174

1,2-Ethanediylbis(oxy)bismethanol, 9CI. 2,5-Dioxa-1,6-hexanediol. Ethylene glycol bis(hemiformal). Dascocide 9

[3586-55-8]

$HOCH_2OCH_2CH_2OCH_2OH$

$C_4H_{10}O_4$ M 122.1

Liq. d^{20} 1.202. n_D^{20} 1.4104.

Belg. Pat., 667 360, (1965); *CA*, **65**, 7002e (*synth*)

U.K. Pat., 997 643, (1965); *CA*, **63**, 11364f (*synth*)

3,3'-Bis(hydroxymethyl) biphenyl B-1-00175

[1,1'-Biphenyl]-3,3'-dimethanol, 9CI

[66888-79-7]

$C_{14}H_{14}O_2$ M 214.2

Needles (CH_2Cl_2). Mp 116.5-117°.

DuVernet, R.B. *et al, J.A.C.S.*, 1978, **100**, 2457 (*synth*)

3,5-Bis(hydroxymethyl) biphenyl B-1-00176

[1,1'-Biphenyl]-3,5-dimethanol, 9CI

[142183-86-6]

$C_{14}H_{14}O_2$ M 214.2

Cryst. ($EtOAc/Et_2O$/petrol). Mp 98-101°.

Müller, W. *et al, Helv. Chim. Acta*, 1992, **75**, 855 (*synth, pmr*)

4,4'-Bis(hydroxymethyl) biphenyl B-1-00177

[1,1'-Biphenyl]-4,4'-dimethanol, 9CI

[1667-12-5]

$C_{14}H_{14}O_2$ M 214.2

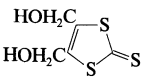
Cryst. Mp 193°.

Weygand, F. *et al, Chem. Ber.*, 1955, **88**, 301 (*synth*)

Sheley, C.T. *et al, Org. Mass Spectrom.*, 1974, **9**, 731 (*synth, ms*)

4,5-Bis(hydroxymethyl)-1,3-dithiole-2-thione, 9CI B-1-00178

[159223-12-8]



$C_5H_6O_2S_3$ M 194.2

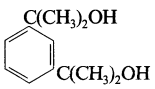
Light yellow needles (Me_2CO/hexane). Mp 86-87°.

Fox, M.A. *et al, J.O.C.*, 1994, **59**, 6519 (*synth, pmr, cmr*)

1,3-Bis(1-hydroxy-1-methylethyl)benzene B-1-00179

α,α,α',α'-Tetramethyl-1,3-benzenedimethanol, 9CI. α,α,α',α'-Tetramethyl-m-*xylene-α,α'-diol, 8CI. α,α'-Dihydroxy*-m-*diisopropylbenzene. 2,2'-*(m-*Phenylene)di-2-propanol*

[1999-85-5]



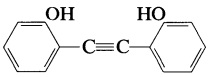
$C_{12}H_{18}O_2$ M 194.2

Cryst. Mp 137-140°.

Johnson, R.A. *et al, Bioorg. Chem.*, 1973, **2**, 99 (*synth, ir, pmr*)

1,2-Bis(2-hydroxyphenyl) acetylene B-1-00180

2,2'-(1,2-Ethynediyl)bisphenol, 9CI. o,o'-*Dihydroxytolan. 2,2'-Tolandiol. 2,2'-Ethynylenediphenol*



$C_{14}H_{10}O_2$ M 210.2

Needles (petrol); cryst. (EtOH aq.). Mp 130-131°.

Di-Me ether: [5293-78-7]. *1,1'-(1,2-Ethynediyl)bis[2-methoxybenzene], 9CI. Bis(2-methoxyphenyl)acetylene. 2,2'-Dimethoxytolan*
$C_{16}H_{14}O_2$ M 238.2 Cryst. (EtOH). Mp 122-124°.

Coleman, G.H. *et al, J.A.C.S.*, 1936, **58**, 2310 (*synth*)

Weygand, C. *et al*, *Ber.*, 1940, **73**, 765 (*di-Me ether*)
Letsinger, R.L. *et al*, *J.A.C.S.*, 1959, **81**, 3013 (*synth*)
Chatt, J. *et al*, *J.C.S.*, 1963, 5170 (*synth*)
Suzuki, T. *et al*, *Chem. Comm.*, 1976, 180 (*di-Me*)
Larock, R.C. *et al*, *J.A.C.S.*, 1984, **106**, 4218 (*di-Me ether*)
Davis, D.S. *et al*, *Acta Cryst. C*, 1993, **49**, 1833 (*cryst struct, di-Me ether*)

1,2-Bis(3-hydroxyphenyl) acetylene B-1-00181

3,3'-(1,2-Ethynediyl)bisphenol, 9CI. m,m'-*Dihydroxytolan. 3,3'-Ethynylenediphenol. 3,3'-Tolandiol*

[161912-04-5]

$C_{14}H_{10}O_2$ M 210.2

Di-Me ether: [59647-77-7]. *1,1'-(1,2-Ethynediyl)bis[3-methoxybenzene], 9CI. Bis(3-methoxyphenyl)acetylene*
$C_{16}H_{14}O_2$ M 238.2 Cryst. Mp 63-63.5°.

Coleman, G.H. *et al*, *J.A.C.S.*, 1936, **58**, 2310 (*di-Me ether*)
Pepermans, H. *et al*, *Bull. Soc. Chim. Belg.*, 1988, **97**, 115 (*trimer*)
Pepermans, H. *et al*, *Magn. Reson. Chem.*, 1988, **26**, 311 (*pmr*)
Cummins, C.H., *Tet. Lett.*, 1994, **35**, 857 (*pmr, cmr*)
Mataka, S. *et al*, *Synthesis*, 1995, 133 (*di-Me ether*)

1,2-Bis(4-hydroxyphenyl) acetylene B-1-00182

4,4'-(1,2-Ethynediyl)bisphenol, 9CI. p,p'-*Dihydroxytolan. 4,4'-Ethynylenediphenol, 8CI. 4,4'-Tolandiol*

[22608-45-3]

$C_{14}H_{10}O_2$ M 210.2
Cryst. (C_6H_6). Mp 214.6-215.1°.

Di-Me ether: [2132-62-9]. *1,1'-(1,2-Ethynediyl)bis[4-methoxybenzene], 9CI. Bis(4-methoxyphenyl)acetylene. 4,4'-Dimethoxytolan*
$C_{16}H_{14}O_2$ M 238.2 Cryst. (EtOH/AcOH). Mp 145-146° (142-143°).

Di-Et ether: [2132-63-0]. *1,1'-(1,2-Ethynediyl) bis[4-ethoxybenzene]. Bis(4-ethoxyphenyl) acetylene. 4,4'-Diethoxytolan*
$C_{18}H_{18}O_2$ M 266.3 Cryst. (EtOH/AcOH). Mp 162-163°.

Dipropyl ether:
$C_{20}H_{22}O_2$ M 294.3 Cryst. (EtOH/AcOH). Mp 133-135°.

Diisopropyl ether:
$C_{20}H_{22}O_2$ M 294.3 Cryst. (EtOH/AcOH). Mp 162-165°.

Dibutyl ether:
$C_{22}H_{26}O_2$ M 322.4 Cryst. (EtOH/AcOH). Mp 127-128°.

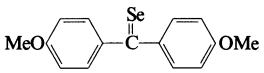
Di-Ph ether: [77384-56-6]. *1,1'-(1,2-Ethynediyl)bis[4-phenoxybenzene], 9CI. 4,4'-Diphenoxytolan*
$C_{26}H_{18}O_2$ M 362.4 Cryst. (C_6H_6). Mp 170-171°.

Tadros, W., *J.C.S.*, 1958, 4210 (*deriv*)
Newman, M.S. *et al*, *J.O.C.*, 1958, **23**, 665 (*di-Me ether*)
Hubacher, M.H., *J.O.C.*, 1959, **24**, 1949 (*synth*)
Greene, F.D. *et al*, *J.A.C.S.*, 1960, **82**, 893 (*di-Me ether*)
Trpin, J. *et al*, *Monatsh. Chem.*, 1969, **100**, 115 (*synth*)
Kaufman, R.J. *et al*, *J.O.C.*, 1982, **47**, 4941 (*synth, di-Me ether, pmr*)
Al-Dujaili, A.H. *et al*, *J. Polym. Sci., Part A: Polym. Chem.*, 1984, **22**, 3127 (*synth, pmr*)
Shioiri, T. *et al*, *Heterocycles*, 1987, **26**, 1467 (*synth*)
Ramana, D.V. *et al*, *Org. Mass Spectrom.*, 1989, **24**, 903 (*ms*)
Pugh, C. *et al*, *J. Polym. Sci., Part A: Polym. Chem.*, 1990, **28**, 1101 (*synth*)

Bis(4-methoxyphenyl) methaneselone B-1-00183

4,4'-Dimethoxyselenobenzophenone

[135655-33-3]



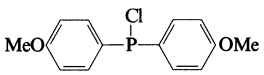
$C_{15}H_{14}O_2Se$ M 305.2
Green needles (pentane). Mp 98-99°.

Okuma, K. *et al*, *J.C.S. Perkin 1*, 1994, 2151 (*synth, cryst struct*)

Bis(4-methoxyphenyl) phosphinous chloride, 9CI B-1-00184

Chlorobis(4-methoxyphenyl)phosphine

[13685-30-8]



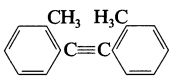
$C_{14}H_{14}ClO_2P$ M 280.6
Solid. Mp 49-53°. Bp_2 190-191°.

Yudina, K.S. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1966, 1954; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1966, 1889.

1,2-Bis(2-methylphenyl) acetylene B-1-00185

1,1'-(1,2-Ethynediyl)bis[2-methylbenzene], 9CI. Di-o-tolylacetylene. 2,2'-Dimethyltolane

[5294-03-1]



$C_{16}H_{14}$ M 206.2
Liq. Bp_5 180-182°. n_D^{20} 1.6228.

Coleman, G.H. *et al*, *J.A.C.S.*, 1936, **58**, 2310 (*synth*)
Merkushev, E.B. *et al*, *Zh. Org. Khim.*, 1982, **18**, 355; *J. Org. Chem. USSR* (*Engl. Transl.*), 1982, **18**, 308 (*synth*)
D'Auria, M., *Synth. Commun.*, 1992, **22**, 2393 (*pmr, cmr, ms*)

1,2-Bis(3-methylphenyl) acetylene B-1-00186

1,1'-(1,2-Ethynediyl)bis[3-methylbenzene], 9CI. Di-m-tolylacetylene. 3,3'-Dimethyltolane

[2765-16-4]

$C_{16}H_{14}$ M 206.2
Cryst. (EtOH or hexane). Mp 74°.

Coleman, G.H. *et al*, *J.A.C.S.*, 1936, **58**, 2310 (*synth*)
Newkome, G.R. *et al*, *J.A.C.S.*, 1980, **45**, 4380 (*synth, pmr, Raman*)
Barba, F. *et al*, *Synth. Commun.*, 1994, **24**, 907 (*synth, ir, pmr, ms*)

1,2-Bis(4-methylphenyl) acetylene B-1-00187

1,1'-(1,2-Ethynediyl)bis[4-methylbenzene], 9CI. Di-p-tolylacetylene. 4,4'-Dimethyltolane

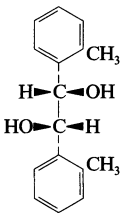
[2789-88-0]

$C_{16}H_{14}$ M 206.2
Cryst. (petrol or AcOH). Mp 136-136.5° (131°). Dimorphic.

Coleman, G.H. *et al*, *J.A.C.S.*, 1934, **56**, 132 (*synth*)
Bader, H. *et al*, *J.A.C.S.*, 1956, **78**, 2590 (*synth*)
Beltrame, P. *et al*, *Gazz. Chim. Ital.*, 1963, **93**, 757 (*uv*)
Horner, L. *et al*, *Chem. Ber.*, 1983, **116**, 1615 (*synth*)

1,2-Bis(2-methylphenyl)-1,2-ethanediol, 9CI B-1-00188

2,2'-Dimethylhydrobenzoin



(*1S,2S*)-*form*

$C_{16}H_{18}O_2$ M 242.3

(***1S,2S***)-***form***
Cryst. (petrol/$CHCl_3$). Mp 109-110°. $[\alpha]_D^{20}$ −72 (c, 1.07 in EtOH) (>98% ee).

(***1RS,2RS***)-***form***
(±)-*form*
Cryst. ($CHCl_3$/petrol). Mp 115° (107-109°).

(***1RS,2SR***)-***form*** [34737-70-7]
meso-*form*
Cryst. (EtOH aq.). Mp 104-105°.

Griffin, G.W. *et al*, *J.O.C.*, 1972, **37**, 2589 (*synth, pmr*)
Raubenheimer, H.G. *et al*, *Chimia*, 1986, **40**, 12 (*synth, pmr*)
Wallace, T.W. *et al*, *J.C.S. Perkin 1*, 1995, 2293 (*synth, pmr, ms*)

Bis(pentafluoroethyl) ether B-1-00189

1,1'-Oxybis[1,1,2,2,2-pentafluoroethane], 9CI. Decafluorodiethyl ether. Perfluorodiethyl ether

[358-21-4]

$F_3CCF_2OCF_2CF_3$

$C_4F_{10}O$ M 254.0
Gas. Bp 2.5°.

U.S. Pat., 2 500 388, (1950); *CA*, **44**, 5236c (*synth*)
Muller, N. *et al*, *J.A.C.S.*, 1957, **79**, 1807 (*F-19 nmr*)
Dresdner, R.D. *et al*, *J.O.C.*, 1959, **24**, 698 (*synth*)

1,2-Bis(pentafluorophenyl)-1,2-diphenyldiphosphine, 8CI B-1-00190

[14655-87-9]

$(C_6F_5)PPh—PPh(C_6F_5)$

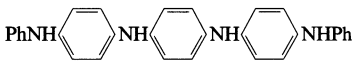
$C_{24}H_{10}F_{10}P_2$ M 550.2
Presumably mixt. of stereoisomers. Cryst. (C_6H_6/petrol). Mp 122-125°.

Fild, M. *et al*, *Naturwissenschaften*, 1967, **54**, 89.

N,N'-Bis[4-(phenylamino) phenyl]-1,4-benzenediamine, 9CI B-1-00191

N-*Phenyltetraaniline*

[19099-70-8]



$C_{30}H_{26}N_4$ M 442.5
Microscopic silver-white cryst. Mp 255-256°.

Ochi, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1994, **67**, 1749.

2,2-Bis(phenylazo)propane B-1-00192

1,1'-(1-Methylethylidene)bis[2-phenyldiazene], 9CI

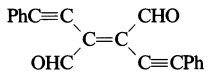
[145729-08-4]

$PhN{=}NC(CH_3)_2N{=}NPh$

$C_{15}H_{16}N_4$ M 252.3
Green-yellow solid (MeOH at −78°). Mp 40° dec.

Engel, P.S. *et al*, *J.O.C.*, 1994, **59**, 6257 (*synth, uv, pmr, cmr*)

2,3-Bis(phenylethynyl) butenedial B-1-00193



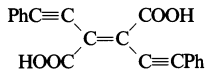
$C_{20}H_{12}O_2$ M 284.3

(*E*)-*form*

2,3-Bis(phenylethynyl)fumaraldehyde
Bright orange solid (hexane). Mp 146°.

Anthony, J. *et al*, *Helv. Chim. Acta*, 1995, **78**, 13.

1,2-Bis(2-phenylethynyl) butenedioic acid B-1-00194



$C_{20}H_{12}O_4$ M 316.3

(*E*)-*form*

Di-Me ester: Dimethyl bis(2-phenylethynyl) fumarate
$C_{22}H_{16}O_4$ M 344.3 Bright yellow cryst. Mp 82°.

Anthony, J. *et al*, *Helv. Chim. Acta*, 1995, **78**, 13.

3,3-Bis(2-phenylethynyl)-1,5-diphenyl-1,4-pentadiyne B-1-00195

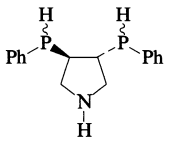
Tetrakis(phenylethynyl)methane

$C(C{\equiv}CPh)_4$

$C_{33}H_{20}$ M 416.5
Solid. Mp 190° dec.

Feldman, K.S. *et al*, *J.A.C.S.*, 1994, **116**, 9019.

3,4-Bis(phenylphosphino) pyrrolidine B-1-00196



$C_{16}H_{19}NP_2$ M 287.2

(*3R,4R*)-*form* [113452-05-4]
Mp 162-165° (as hydrochloride). $[\alpha]_D^{23}$ −76 (c, 2.68 in EtOH). Mixt. of diastereoisomers at the two P atoms.

1-Benzyl: [113452-11-2].
$C_{23}H_{25}NP_2$ M 377.4 $[\alpha]_D^{23}$ −47 (c, 1.33 in MeOH) (as hydrochloride).

1-tert-*Butoxycarbonyl:*
$C_{21}H_{27}NO_2P_2$ M 387.3 Oil.
Characterised as $PdCl_2$ complex.

[113452-08-7, 113452-14-5]

Nagel, U. *et al*, *Chem. Ber.*, 1988, **121**, 1123; 1992, **125**, 1061 (*synth, ir, ms, pmr, P-31 nmr*)

Bis(phenylseleno)methane B-1-00197

1,1'-[Methylenebis(seleno)]bisbenzene, 9CI

[20343-90-2]

$PhSeCH_2SePh$

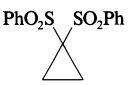
$C_{13}H_{12}Se_2$ M 326.1
Cryst. (EtOH or hexane/Et_2O). Mp 36-38° (30-30.6°). $Bp_{0.1}$ 138°.

Petragnani, N. *et al*, *Chem. Ber.*, 1970, **103**, 2271 (*synth*)
Seebach, D. *et al*, *Chem. Ber.*, 1972, **105**, 511 (*synth, ir, pmr, uv*)
Reich, H.J. *et al*, *J.O.C.*, 1979, **101**, 6638 (*synth, pmr*)
Engman, L. *et al*, *Synthesis*, 1980, 569 (*synth*)
Levason, W. *et al*, *J.C.S. Perkin 2*, 1984, 429 (*synth, ms*)
Duddeck, H. *et al*, *Magn. Reson. Chem.*, 1993, **31**, 736 (*cmr, pmr, Se-77 nmr*)
Silveira, C.C. *et al*, *Synth. Commun.*, 1995, **25**, 117 (*synth, pmr, ms*)

1,1-Bis(phenylsulfonyl) cyclopropane B-1-00198

1,1'-[Cyclopropylidenebis(sulfonyl)]bisbenzene, 9CI

[34782-46-2]



$C_{15}H_{14}O_4S_2$ M 322.4
Source of propylene 1,3-dipole. Mp 149° (145-146°).

Becker, G. *et al*, *Tet. Lett.*, 1971, 4081 (*synth*)
Trost, B.M. *et al*, *J.A.C.S.*, 1983, **105**, 1052 (*synth, cmr*)
Rao, Y.K. *et al*, *Indian J. Chem., Sect. B*, 1986, **25**, 1031 (***synth***)
Benedetti, F. *et al*, *J.C.S. Perkin 2*, 1986, 605 (*synth*)
Benedetti, F. *et al*, *Org. Mass Spectrom.*, 1988, **23**, 573 (*ms*)

Bis(phenylsulfonyl)sulfide B-1-00199

Benzenesulfanothioic acid anhydrosulfide, 9CI. Benzenesulfonyl sulfide

[4388-22-1]

$PhSO_2SSO_2Ph$

$C_{12}H_{10}O_4S_3$ M 314.4
Prisms (AcOH). Insol. H_2O. Mp 136-137° (133°).

Mathieson, A.M. *et al*, *J.C.S.*, 1948, 322; 1949, 724 (*synth, cryst struct*)
Hayashi, S. *et al*, *Chem. Pharm. Bull.*, 1967, **15**, 1310 (*synth*)
Abe, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 3678.
Mizhiritskii, M.D. *et al*, *Zh. Obshch. Khim.*, 1986, **56**, 1547; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1986, **56**, 1373 (*synth*)

Bis(phenylthio)acetaldehyde B-1-00200

[153823-24-6]

$(PhS)_2CHCHO$

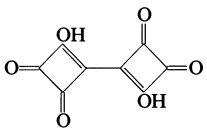
$C_{14}H_{12}OS_2$ M 260.3
Unstable, can be stored in refrigerator.

Ishibashi, H. *et al*, *J.O.C.*, 1995, **60**, 1276 (*synth, pmr*)

Bisquaric acid B-1-00201

2,2'-Dihydroxy[bi-1-cyclobuten-1-yl]-3,3',4,4'-tetrone, 9CI. 4,4'-Bi(3-hydroxy-3-cyclobutene-1,2-dione)

[152931-71-0]



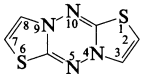
$C_8H_2O_6$ M 194.1
Bright yellow cryst. Sol. H_2O and DMSO; insol. most other org. solvs. Mp >270°. pK_a −4.49.

Diisopropyl ether: [152931-80-1].
$C_{14}H_{14}O_6$ M 278.2 Orange solid (CH_2Cl_2/hexane). Mp 124-125°.

Liebeskind, L.S. *et al*, *J.A.C.S.*, 1993, **115**, 9048 (*synth, cryst struct, ir, cmr, pmr*)

Bisthiazolo[3,2-*b*:3',2'-*e*][1,2,4,5]tetrazine, 9CI B-1-00202

[154353-45-4]



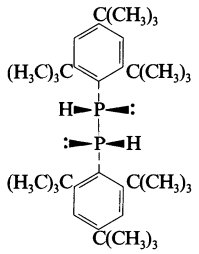
$C_6H_4N_4S_2$ M 196.2
Orange-yellow needles. Dec. slowly above 150° without melting.

Stumpf, M. *et al*, *Annalen*, 1994, 1049 (*synth, uv, pmr*)

1,2-Bis(2,4,6-tri-*tert*-butylphenyl)diphosphine, 8CI B-1-00203

1,2-Bis[2,4,6-tris(1,1-dimethylethyl)phenyl] diphosphine, 9CI. 1,2-Disupermesityldiphosphine

[83115-14-4]



(*1RS,2RS*)-*form*

$C_{36}H_{60}P_2$ M 554.8

(***1RS,2RS*)-*form*** [86539-29-9]
(±)-*form*
Solid. Mp 147-148.5°.

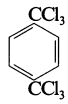
(***1RS,2SR*)-*form*** [86539-30-2]
meso-*form*
Not. obt. pure.

Cowley, A.H. *et al*, *J.A.C.S.*, 1982, **104**, 5820; 1984, **106**, 1491 (*synth, pmr, P-31 nmr, props*)
Yoshifuji, M. *et al*, *Chem. Lett.*, 1983, 585 (*synth, P-31 nmr*)

1,4-Bis(trichloromethyl) benzene, 9CI B-1-00204

α,α,α,α',α',α'-Hexachloro-p-xylene, 8CI. Hexachlorxylol. Bitriben. Chloxyl. Getol. Hetol Hoechst. Khloksil. WR 17206

[68-36-0]

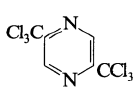


$C_8H_4Cl_6$ M 312.8
Fasciolicide, antimalarial agent. Cryst. (hexane). Mp 108-110°.

▶ LD_{50} (rat, orl) 3200 mg/kg. Exp. reprod. effects. Hepatotoxic. ZE4655000.

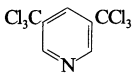
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, **2**, 150B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 999A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 918C (*ir*)
Ross, S.D. *et al*, *J.A.C.S.*, 1953, **75**, 4967 (*synth*)
Aviado, D.M. *et al*, *Exp. Parasitol.*, 1969, **25**, 283 (*pharmacol*)
Elslager, E.F. *et al*, *J. Med. Chem.*, 1970, **13**, 542 (*activity*)
Genther, C.S. *et al*, *J. Med. Chem.*, 1977, **20**, 237 (*activity*)
Hamada, K. *et al*, *Acta Cryst. C*, 1987, **43**, 953 (*cryst struct*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, HCM500.

2,5-Bis(trichloromethyl) pyrazine B-1-00205



$C_6H_2Cl_6N_2$ M 314.8
Cryst. (2-butanone). Mp 173-177°.
Cartwright, D. *et al*, *J.C.S. Perkin 1*, 1995, 2595 (*synth, pmr, cmr*)

3,5-Bis(trichloromethyl) pyridine B-1-00206

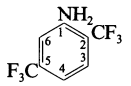


$C_7H_3Cl_6N$ M 313.8
Solid. Mp 78-79°.
Cartwright, D. *et al*, *J.C.S. Perkin 1*, 1995, 2595 (*synth, pmr*)

2,5-Bis(trifluoromethyl)aniline B-1-00207

2,5-Bis(trifluoromethyl)benzenamine, 9CI. α,α,α,α',α',α'-Hexafluoro-2,5-xylidine

[328-93-8]



$C_8H_5F_6N$ M 229.1
Liq. d_{20}^4 1.47. Bp 173-177°, $Bp_{14.5}$ 70.5°. n_D^{20} 1.4322.

N-*Ac:*
$C_{10}H_7F_6NO$ M 271.1 Cryst. (EtOH). Mp 146.5-147°.

U.S. Pat., 2 432 393, (1943); *CA*, **42**, 2441f (*synth*)
Ross, S.D. *et al*, *J.A.C.S.*, 1953, **75**, 4967 (*synth, Ac*)
Yates, K. *et al*, *Can. J. Chem.*, 1972, **50**, 581 (*synth*)

3,5-Bis(trifluoromethyl)aniline B-1-00208

3,5-Bis(trifluoromethyl)benzenamine. α,α,α,α',α',α'-Hexafluoro-3,5-xylidine

[328-74-5]

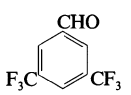
$C_8H_5F_6N$ M 229.1
d_{20}^4 1.47. Bp_{15} 85°.

[90269-60-6]

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1149D.
Aldrich Library of NMR Spectra, 2nd edn., **1**, 1040B.
Maginnity, P.M. *et al*, *J.A.C.S.*, 1951, **73**, 3579 (*synth*)
Ross, S.D. *et al*, *J.A.C.S.*, 1953, **75**, 4967 (*synth*)

3,5-Bis(trifluoromethyl) benzaldehyde, 9CI B-1-00209

[401-95-6]



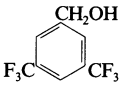
$C_9H_4F_6O$ M 242.1
Oil. Bp_3 50°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1303C.
Krishnamurthy, V.V. *et al*, *J.A.C.S.*, 1984, **106**, 7068 (*cmr*)
Blackburn, C. *et al*, *J.A.C.S.*, 1985, **107**, 2442 (*synth*)
Schaefer, T. *et al*, *Can. J. Chem.*, 1989, **67**, 827 (*synth, pmr*)

3,5-Bis(trifluoromethyl) benzenemethanol, 9CI B-1-00210

3,5-Bis(trifluoromethyl)benzyl alcohol, 8CI

[32707-89-4]



$C_9H_6F_6O$ M 244.1
Mp 54-56°.

U.K. Pat., 1 214 109, (1970); *CA*, **75**, 5910e.
U.S. Pat., 3 625 971, (1971); *CA*, **76**, 59617d.
Blackburn, C. *et al*, *J.A.C.S.*, 1985, **107**, 2442 (*synth, pmr, ir, ms*)

1,1-Bis(trifluoromethyl) diphosphine, 9CI, 8CI B-1-00211

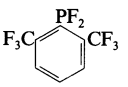
[33974-71-9]

$C_2H_2F_6P_2$ M 201.9
Liq. at −95°. Bp 75° (extrap.). Shows 4% dec. after 1 day at 0°.

Demuth, R. *et al*, *Z. Naturforsch., B*, 1971, **26**, 731 (*synth, pmr, F-19 nmr, P-31 nmr*)
Demuth, R. *et al*, *J. Fluorine Chem.*, 1973, **2**, 269, 299 (*synth, pmr, reactions, F-19 nmr, P-31 nmr*)

[2,6-Bis(trifluoromethyl) phenyl]phosphonous difluoride B-1-00212

[152508-66-2]

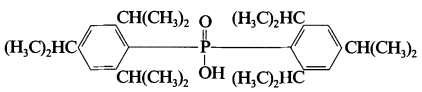


$C_8H_3F_8P$ M 282.0
Liq. Bp_7 70°.

Meyer, T.G. *et al*, *Z. Naturforsch., B*, 1993, **48**, 875 (*synth, ms, cmr, F-19 nmr, P-31 nmr*)

Bis(2,4,6-triisopropylphenyl) phosphinic acid B-1-00213

Bis[2,4,6-tris(1-methylethyl)phenyl]phosphinic acid



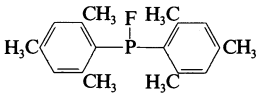
$C_{30}H_{47}O_2P$ M 470.6
Chloride: [147050-16-6].
$C_{30}H_{46}ClOP$ M 489.1 Waxy solid.
Azide: [137248-26-1].
$C_{30}H_{46}N_3OP$ M 495.6 Cryst. (MeOH). Mp 81-82.5°.

Harger, M.J.P. *et al*, *J.C.S. Perkin 1*, 1993, 227 (*synth, ms, ir, pmr, P-31 nmr*)

Bis(2,4,6-trimethylphenyl) phosphinous fluoride, 9CI B-1-00214

Dimesitylphosphinous fluoride, 8CI. Fluorodimesitylphosphine

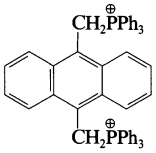
[152508-64-0]



$C_{18}H_{22}FP$ M 288.3
Liq. $Bp_{0.6}$ 56°.
Meyer, T.G. *et al*, *Z. Naturforsch., B*, 1993, **48**, 875 (*synth, F-19 nmr, P-31 nmr*)

9,10-Bis (triphenylphosphinomethyl) anthracene(2+) B-1-00215

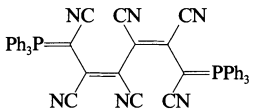
[9,10-Anthracenediylbis(methylene)] bis[triphenylphosphonium]



$C_{52}H_{42}P_2^{2\oplus}$ M 728.8 (ion)
Dichloride: [10273-81-1].
$C_{52}H_{42}Cl_2P_2$ M 799.7 Yellow cryst. (DMF). Sol. alcohols, CH_2Cl_2; spar. sol. $CHCl_3$; insol. C_6H_6, toluene, aliphatic hydrocarbons. Mp 280° dec. Exhibits blue-violet fluor.
Listvan, V.N., *Zh. Obshch. Khim.*, 1985, **55**, 2629; *J. Gen. Chem. USSR (Engl. Transl.)*, 1985, **55**, 2337 (*synth, props*)
Claerebondt, J. *et al*, *Org. Mass Spectrom.*, 1993, **28**, 71 (*ms*)

1,6-Bis(triphenylphosphoranylidene)-2,4-hexadiene-1,2,3,4,5,6-hexacarbonitrile B-1-00216

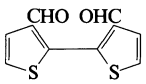
1,2,3,4,5,6-Hexacyano-1,6-bis(triphenylphosphoranylidene)-2,4-hexadiene
[18629-15-7]



$C_{48}H_{30}N_6P_2$ M 752.7
Adduct from Ph_3P and NCC≡CCN. Orange-red cryst. (Py or MeCN). Mp 237-239°.
Reddy, G.S. *et al*, *J.O.C.*, 1963, **28**, 1822 (*synth, ir, uv*)
Shaw, M.A. *et al*, *J.C.S.(C)*, 1968, 1609 (*ir, ms, uv, pmr*)
Butterfield, P.J. *et al*, *J.C.S. Perkin 1*, 1978, 1237 (*cryst struct*)

[2,2′-Bithiophene]-3,3′-dicarboxaldehyde, 9CI B-1-00217

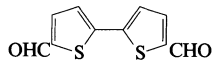
3,3′-Diformyl-2,2′-bithienyl
[19690-70-1]



$C_{10}H_6O_2S_2$ M 222.2
Brown plates (C_6H_6). Mp 156-158°.
Yoshida, S. *et al*, *J.O.C.*, 1994, **59**, 3077 (*synth, ir, pmr*)

[2,2′-Bithiophene]-5,5′-dicarboxaldehyde B-1-00218

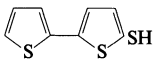
5,5′-Diformyl-2,2′-bithienyl
[32364-72-0]



$C_{10}H_6O_2S_2$ M 222.2
Yellow plates (C_6H_6/petrol). Mp 217-218°.
Curtis, R.F. *et al*, *Tetrahedron*, 1967, **23**, 4419 (*synth, uv, ir*)

[2,2′-Bithiophene]-5-thiol, 9CI B-1-00219

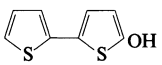
5-Mercapto-2,2′-bithiophene
[159157-32-1]



$C_8H_6S_3$ M 198.3
Liq. Mp 20°. $Bp_{0.1}$ 95°.
Purcell, S.T. *et al*, *J.A.C.S.*, 1994, **116**, 11985 (*synth, pmr*)
Effenberger, F. *et al*, *J.O.C.*, 1995, **60**, 2082 (*synth, pmr*)

2,2′-Bithiophen-5-ol B-1-00220

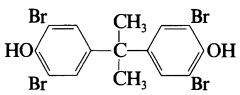
5-Hydroxy-2,2′-bithiophene



$C_8H_6OS_2$ M 182.2
Me ether: 5-Methoxy-2,2′-bithiophene
$C_9H_8OS_2$ M 196.2 Yellow oil. $Bp_{0.1}$ 90°.
Effenberger, F. *et al*, *J.O.C.*, 1995, **60**, 2082 (*synth, pmr*)

Bromdian B-1-00221

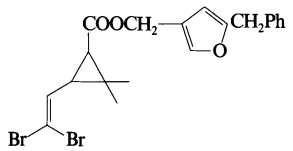
4,4′-(1-Methylethylidene)bis[2,6-dibromophenol], *9CI. 4,4′-Isopropylidenebis[2,6-dibromophenol]*, *8CI. 2,2-Bis(3,5-dibromo-4-hydroxyphenyl)propane. Tetrabromobisphenol A*
[79-94-7]



$C_{15}H_{12}Br_4O_2$ M 543.8
Flame retardant. Monomer. Cryst. Mp 161-162°.
Kohn, M., *Monatsh. Chem.*, 1931, **58**, 108 (*synth*)
Holahan, F.S. *et al*, *Makromol. Chem.*, 1967, **103**, 36 (*synth*)
Islam, A.M. *et al*, *Egypt. J. Chem.*, 1977, **20**, 483 (*synth*)
Simonov, Yu.A. *et al*, *Kristallografiya*, 1986, **31**, 397; *CA*, **104**, 197560c (*cryst struct*)

Bromethirin B-1-00222

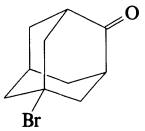
[5-(Phenylmethyl)-3-furanyl]methyl 3-(2,2-dibromoethenyl)-2,2-dimethylcyclopropanecarboxylate, *9CI*
[42789-03-7]



$C_{20}H_{20}Br_2O_3$ M 468.1
(1*R*,3*R*)- and (1*R*,3*S*)-isomers reported. No phys. data given. Insecticide.
[42789-04-8, 49550-79-0, 56194-80-0, 65167-03-5, 65167-13-7]
Elliott, M. *et al*, *J.C.S. Perkin 1*, 1974, 2470.
Elliott, M. *et al*, *Pestic. Sci.*, 1975, **6**, 537 (*synth, use*)
Jones, N.F., *J.C.S. Perkin 1*, 1977, 1878 (*cmr*)

5-Bromo-2-adamantanone B-1-00223

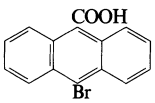
5-Bromotricyclo[3.3.1.1^{3,7}]decanone, *9CI*
[20098-20-8]



$C_{10}H_{13}BrO$ M 229.1
Cryst. (petrol). Mp 150-154°.
Geluk, H.W. *et al*, *Tetrahedron*, 1968, **24**, 5369 (*synth, pmr, ir*)

10-Bromo-9-anthracenecarboxylic acid, 9CI B-1-00224

10-Bromo-9-anthroic acid, *8CI*
[6929-81-3]



$C_{15}H_9BrO_2$ M 301.1
Yellow cryst. (AcOH or EtOH). Mp 273° dec., (265-267° dec.). pK_a 4.09 (50% EtOH aq. at 25°).
Me ester:
$C_{16}H_{11}BrO_2$ M 315.1 Yellow needles (MeOH). Mp 114-115°.
Et ester:
$C_{17}H_{13}BrO_2$ M 329.1 Yellow needles. Mp 83°.
Nitrile: [80393-52-8]. *9-Bromo-10-cyanoanthracene*
$C_{15}H_8BrN$ M 282.1 Oil.
Beyer, H. *et al*, *Ber.*, 1941, **74**, 494 (*synth, esters*)
Parish, R.C. *et al*, *J.O.C.*, 1965, **30**, 927 (*Me ester*)
Anderson, G.L. *et al*, *J.A.C.S.*, 1971, **93**, 6984 (*props*)
Inouye, M. *et al*, *J.A.C.S.*, 1993, **115**, 8091 (*nitrile, synth, ir, pmr, cmr*)

5-Bromo-1,3-benzenedicarboxylic acid B-1-00225

5-Bromoisophthalic acid

[23351-91-9]

$C_8H_5BrO_4$ M 245.0
Needles (Me_2CO aq.). Mp 282-283°.

Diamide:
$C_8H_7BrN_2O_2$ M 243.0 Fine needles. Mp 293-294° dec.

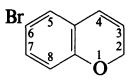
Dinitrile: 2-Bromo-1,3-dicyanobenzene
$C_8H_3BrN_2$ M 207.0 Fine needles. Mp 128-130°.

Crandall, E.W. *et al, Org. Prep. Proced. Int.*, 1969, **1**, 147 (*synth*)
Doyle, T.J. *et al, J. Het. Chem.*, 1994, **31**, 1417 (*diamide, dinitrile*)

6-Bromo-2*H*-1-benzopyran, 9CI, 8CI B-1-00226

*6-Bromo-3-chromene. 6-Bromo-2*H*-chromene*

[18385-87-0]



C_9H_7BrO M 211.0
Bp_{14} 136°, Bp_1 80°. n_D^{20} 1.6202.

Maitte, P., *Ann. Chim. (Paris)*, 1954, **9**, 431 (*synth*)
Canalini, G. *et al, Ann. Chim. (Rome)*, 1967, **57**, 1045 (*synth, uv, pmr*)
Sliwa, H. *et al, Synthesis*, 1993, 881 (*synth, pmr, cmr*)

7-Bromo-2*H*-1-benzopyran, 8CI B-1-00227

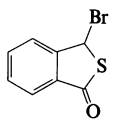
*7-Bromo-2*H*-chromene*

[18385-92-7]

C_9H_7BrO M 211.0
$Bp_{0.6}$ 91-92°. n_D^{23} 1.6029.

Canalini, G. *et al, Ann. Chim. (Rome)*, 1967, **57**, 1045 (*synth, uv, pmr*)

3-Bromobenzo[*c*]thiophen-1(3*H*)-one B-1-00228



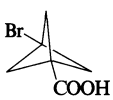
C_8H_5BrOS M 229.0

(±)-***form*** [155988-84-4]
Cryst. (C_6H_6/petrol). Mp 82-84°.

Majumdar, G. *et al, J.C.S. Perkin 1*, 1994, 309.

3-Bromobicyclo[1.1.1]pentane-1-carboxylic acid, 9CI B-1-00229

[156329-70-3]



$C_6H_7BrO_2$ M 191.0
Cryst. (Et_2O/pentane). Mp 176-178°.

Na salt: [156329-60-1].
Solid.

Me ester: [83249-14-3].
$C_7H_9BrO_2$ M 205.0 Cryst. Mp 49-50°.

Nitrile: [156329-61-2]. *1-Bromo-3-cyanobicyclo[1.1.1]pentane*
C_6H_6BrN M 172.0 Cryst. by subl. Mp 119-120°.

Applequist, D.E. *et al, J.O.C.*, 1982, **47**, 4985 (*Me ester, synth, ir*)
Della, E.W. *et al, J.O.C.*, 1994, **59**, 2986 (*synth, pmr, cmr, ms*)

Bromobis(trifluoromethyl) arsine, 8CI B-1-00230

Bis(trifluoromethyl)arsinous bromide, 9CI. Bis(trifluoromethyl)arsenic bromide

[359-52-4]

$(F_3C)_2AsBr$

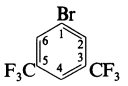
C_2AsBrF_6 M 292.8
Synth. from $(F_3C)_3As + Br_2$ at −5°. Liq. Bp_{745} 59.5°. n_D^{20} 1.398. Treatment with aq. alkali gives F_3CH.

Emeléus, H.J. *et al, J.C.S.*, 1953, 1552 (*synth, props*)
Demuth, R., *Z. Anorg. Allg. Chem.*, 1975, **418**, 149 (*ir, Raman*)

1-Bromo-3,5-bis(trifluoromethyl)benzene, 9CI B-1-00231

*5-Bromo-α,α,α,α′,α′,α′-hexafluoro-*m*-xylene, 8CI*

[328-70-1]



$C_8H_3BrF_6$ M 293.0
d_4^{25} 1.699. Mp −16°. Bp 153.9°. n_D^{25} 1.4241, (1.4250).

Mcbee, E.T. *et al, J.A.C.S.*, 1950, **72**, 1651 (*synth, props*)
Urban, J. *et al, Coll. Czech. Chem. Comm.*, 1987, **52**, 1340 (*synth*)

4-Bromo-1,3-bis(trifluoromethyl)benzene, 9CI B-1-00232

2,4-Bis(trifluoromethyl)-1-bromobenzene

[327-75-3]

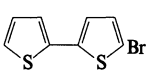
$C_8H_3BrF_6$ M 293.0
d^{20} 1.74. Bp 161.5°. n_D^{20} 1.6363.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 932A.
U.S. Pat., 4 388 472, (1983); *CA*, **99**, 122041d.
Kodaira, K. *et al, Bull. Chem. Soc. Jpn.*, 1988, **61**, 1625.

5-Bromo-2,2′-bithiophene, 9CI B-1-00233

5-Bromo-2,2′-bithienyl

[3480-11-3]



$C_8H_5BrS_2$ M 245.1
Solid (MeOH). Mp 34°. $Bp_{0.04}$ 89-91°.

Curtis, R.F. *et al, J.C.S.*, 1965, 5134 (*synth, uv*)
Carpita, A. *et al, Gazz. Chim. Ital.*, 1985, **115**, 575 (*synth, cmr*)
Zimmer, H. *et al, Phosphorus Sulfur Relat. Elem.*, 1989, **46**, 153 (*synth, pmr, ms*)
Bäuerle, P. *et al, Synthesis*, 1993, 1099 (*synth, pmr*)

1-Bromo-2-(bromomethyl)-2-butylamine B-1-00234

2-Amino-1,3-dibromo-2-ethylpropane

$(BrCH_2)_2C(NH_2)CH_2CH_3$

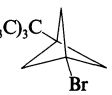
$C_5H_{11}Br_2N$ M 244.9
Hydrobromide: [24083-55-4].
Microcryst. solid (EtOH aq.). Mp 234-235° (230°).

Funke, W., *Chem. Ber.*, 1969, **102**, 3148 (*synth*)
Marchand, A.P. *et al, J.O.C.*, 1994, **59**, 1608 (*synth*)

1-Bromo-3-*tert*-butylbicyclo[1.1.1]pentane B-1-00235

1-Bromo-3-(1,1-dimethylethyl)bicyclo[1.1.1]pentane, 9CI

[127321-07-7]



$C_9H_{15}Br$ M 203.1
Cryst. by subl. Mp 83-84° (80.5-81°).

Kaszynskii, P. *et al, J.A.C.S.*, 1992, **114**, 601 (*synth, pmr, cmr, ir, ms*)
Della, E.W. *et al, J.O.C.*, 1994, **59**, 2986 (*synth, pmr, cmr, ms*)

1-Bromo-3-chlorobicyclo[1.1.1]pentane, 9CI B-1-00236

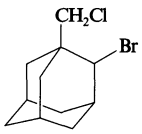
[155635-19-1]

C_5H_6BrCl M 181.4
Cryst. by subl. Mp 84°.

Della, E.W. *et al, J.O.C.*, 1994, **59**, 2986 (*synth, pmr, cmr, ms*)

2-Bromo-1-(chloromethyl) adamantane B-1-00237

[157490-72-7]

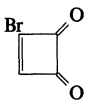


$C_{11}H_{16}BrCl$ M 263.6

Mlinarić-Majerski, K. *et al, J.O.C.*, 1994, **59**, 4362 (*synth, pmr, cmr, ms*)

3-Bromo-3-cyclobutene-1,2-dione B-1-00238

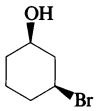
Semisquaric acid bromide



C_4HBrO_2 M 160.9
Yellow oil. $Bp_{0.037}$ 64°.

Schmidt, A.H. *et al*, *Synthesis*, 1994, 422 (*synth, ir, pmr, cmr, ms*)

3-Bromocyclohexanol B-1-00239



$C_6H_{11}BrO$ M 179.0
Parent compd. not descr. (1995).

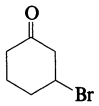
(1RS,3SR)-form
(±)-cis-*form*

Ac: [58268-53-4].
$C_8H_{13}BrO_2$ M 221.0 Liq.

Saloman, R.G. *et al*, *J.O.C.*, 1976, **41**, 1529 (*synth, pmr, ms, deriv*)

3-Bromocyclohexanone, 9CI B-1-00240

[62784-60-5]

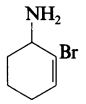


C_6H_9BrO M 177.0
Not isol. No phys. data given. V. sensitive to loss of HBr.

Grenier-Loustalot, M.F. *et al*, *Spectrochim. Acta A*, 1976, **32**, 1743 (*ir*)
Marx, J.N., *Tetrahedron*, 1983, **39**, 1529 (*synth, pmr*)
Bowen, J.P. *et al*, *J.O.C.*, 1987, **52**, 1830 (*conformn*)

2-Bromo-2-cyclohexen-1-amine B-1-00241

6-Amino-1-bromocyclohexene



$C_6H_{10}BrN$ M 176.0

(±)-form [161196-42-5]
Light brown oil.

Banwell, M.G. *et al*, *Aust. J. Chem.*, 1994, **47**, 2235 (*synth, pmr, cmr*)

2-Bromo-1,1,1,3,3,4,4,5,5,5-decafluoro-2-(trifluoromethyl)pentane, 9CI, 8CI B-1-00242

[22528-67-2]

$F_3CCF_2CF_2C(CF_3)_2Br$

C_6BrF_{13} M 398.9
Bp 99-101°.

Miller, W.T. *et al*, *J.A.C.S.*, 1968, **90**, 7367 (*synth*)
Smart, B.E. *et al*, *J.A.C.S.*, 1986, **108**, 4905 (***synth***, *ms, nmr, ir*)

10-Bromodecanal, 9CI B-1-00243

[85920-81-6]

$BrCH_2(CH_2)_8CHO$

$C_{10}H_{19}BrO$ M 235.1
Oil. Bp_3 128-130°. n_D^{20} 1.4710; oxid. in air.

Semicarbazone: Cryst. (EtOH aq.). Mp 85.5-86.5°.

Chuit, P. *et al*, *Helv. Chim. Acta*, 1926, **9**, 1074 (*synth*)
Sorochinskaya, A.M. *et al*, *Khim. Prir. Soedin.*, 1989, 264; *Chem. Nat. Compd. (Engl. Transl.)*, 1989, 228 (*synth*)
Bestmann, H.J. *et al*, *Synthesis*, 1994, 1257 (*synth, pmr*)

10-Bromo-1-decene, 9CI B-1-00244

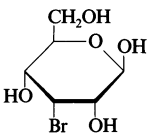
[62871-09-4]

$H_2C{=}CH(CH_2)_7CH_2Br$

$C_{10}H_{19}Br$ M 219.1
Liq. Bp_{55} 149-150°. n_D^{20} 1.4703.

Fréchet, J.M.J. *et al*, *J.A.C.S.*, 1992, **114**, 6630 (*synth, pmr*)
Percec, V. *et al*, *Macromolecules*, 1993, **26**, 3663 (*synth, pmr*)
Johnson, D.K. *et al*, *Synth. Commun.*, 1994, **24**, 1557 (*synth, pmr, cmr*)

3-Bromo-3-deoxyallose B-1-00245



β-D-Pyranose-*form*

$C_6H_{11}BrO_5$ M 243.0

β-D-Pyranose-form

Tetra-Ac: [106023-35-2].
$C_{14}H_{19}BrO_9$ M 411.2 Syrup. $[\alpha]_D^{20}$ −14.1 (c, 1.6 in $CHCl_3$).

Me glycoside: [127236-54-8].
$C_7H_{13}BrO_5$ M 257.0 Syrup.

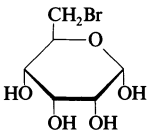
Me glycoside, 4,6-O-benzylidene: [77842-63-8].
$C_{14}H_{17}BrO_5$ M 345.1 Cryst. (EtOAc/petrol). Mp 120-122° (97-99°). $[\alpha]_D^{22}$ −9 (c, 1.5 in $CHCl_3$), $[\alpha]_D^{22}$ −23 ($CHCl_3$).

α-D-Furanose-form

1,2:5,6-Di-O-isopropylidene: [74958-56-8].
$C_{12}H_{19}BrO_5$ M 323.1 Cryst. (pentane). Mp 45°. $[\alpha]_D^{22}$ +55 (c, 1.5 in $CHCl_3$).

Bundle, D. *et al*, *J.C.S. Perkin 1*, 1979, 2751 (*β-Me pyr benzylidene, pmr*)
Classon, B. *et al*, *Can. J. Chem.*, 1981, **59**, 339 (*β-Me pyr benzylidene*)
Kunz, H.Y. *et al*, *Annalen*, 1982, 1245 (*α-diisopropylidene*)
Korth, H.G. *et al*, *J.C.S. Perkin 2*, 1986, 1461 (*β-tetra-Ac, pmr*)
Krylova, R.G. *et al*, *Bioorg. Khim.*, 1990, **16**, 105; *Sov. J. Bioorg. Chem. (Engl. Transl.)*, 1990, **16**, 56 (*β-Me pyr derivs, pmr*)

6-Bromo-6-deoxyallose B-1-00246



$C_6H_{11}BrO_5$ M 243.0

α-D-Pyranose-form

Me glycoside, 4-benzoyl: [52572-05-1].
$C_{14}H_{17}BrO_6$ M 361.1 Syrup.

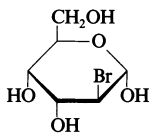
Me glycoside, 4-benzoyl, 2,3-di-Ac: [116013-31-1].
$C_{18}H_{21}BrO_8$ M 445.2 Syrup. $[\alpha]_D$ +42 ($CHCl_3$).

Me glycoside, 4-benzoyl, 2,3-di-Me: [22893-89-6].
$C_{16}H_{21}BrO_6$ M 389.2 Syrup. $[\alpha]_D$ +95 (c, 0.5 in $CHCl_3$).

Me glycoside, 4-benzoyl, 2,3-anhydro: [18933-59-0].
$C_{14}H_{15}BrO_5$ M 343.1 Cryst. (EtOAc/hexane). Mp 60-61° (55°). $[\alpha]_D$ +177 ($CHCl_3$).

Brimacombe, J.S. *et al*, *Chem. Comm.*, 1969, 197 (*di-Me, ir*)
Baer, H.H. *et al*, *Carbohydr. Res.*, 1973, **28**, 390 (*anhydro*)
Collins, P.M. *et al*, *Carbohydr. Res.*, 1974, **33**, 25 (*4-benzoyl, ir*)
Chana, J.S. *et al*, *Chem. Comm.*, 1988, 94 (*di-Ac, pmr*)
Chretien, F. *et al*, *Synth. Commun.*, 1990, **20**, 1589 (*anhydro*)

2-Bromo-2-deoxyaltrose B-1-00247



α-D-Pyranose-*form*

$C_6H_{11}BrO_5$ M 243.0

α-D-Pyranose-form

Me glycoside:
$C_7H_{13}BrO_5$ M 257.0 Cryst. (EtOH). Mp 153°. $[\alpha]_D$ +86.2 (c, 0.5 in EtOH).

Me glycoside, 4,6-O-benzylidene: [19465-09-9].
$C_{14}H_{17}BrO_5$ M 345.1 Cryst. (Me_2CO/hexane). Mp 117-118°. $[\alpha]_D^{25}$ +59.2 (c, 1.0 in $CHCl_3$).

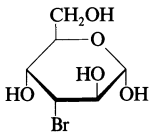
Me glycoside, 3,4-O-isopropylidene:
$C_{10}H_{17}BrO_5$ M 297.1 Mp 64-66°. $[\alpha]_D$ +43.1 ($CHCl_3$).

β-D-Pyranose-form

1,6-Anhydro, 3,4-di-Ac:
$C_{10}H_{13}BrO_6$ M 309.1 Syrup. $Bp_{0.01}$ 160-190° (bath). $[\alpha]_D^{20}$ −68 (in $CHCl_3$).

Newth, F.H. *et al*, *J.C.S.*, 1947, 10 (*anhydro, di-Ac*)
Richards, G.N. *et al*, *J.C.S.*, 1953, 2442 (*Me gly, benzylidene*)
Sharma, M. *et al*, *Can. J. Chem.*, 1968, **46**, 757 (*benzylidene, ir, pmr*)
Guindon, Y. *et al*, *J.O.C.*, 1987, **52**, 1680 (*benzylidene*)

3-Bromo-3-deoxyaltrose B-1-00248



$C_6H_{11}BrO_5$ M 243.0

α-D-Pyranose-form

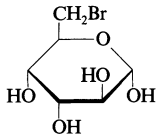
Me glycoside, 4,6-O-benzylidene: $C_{14}H_{17}BrO_5$ M 345.1 Cryst. Mp 123-124°. $[\alpha]_D$ +120 ($CHCl_3$).

Me glycoside, 4,6-O-benzylidene, 2-Ac: [20853-48-9]. $C_{16}H_{19}BrO_6$ M 387.2 Cryst. ($CHCl_3$/petrol). Mp 101-103°. $[\alpha]_D^{20}$ +80.5 (c, 1.0 in $CHCl_3$).

Me glycoside, 4,6-O-benzylidene, 2-benzoyl: [55169-78-3]. $C_{21}H_{21}BrO_6$ M 449.2 Cryst. (EtOAc/pentane). Mp 136.5-138°. $[\alpha]_D^{21}$ +1.6 (c, 1.5 in $CHCl_3$).

Lee, J.B. *et al, Tetrahedron*, 1961, **12**, 226 (*Me gly benzylidene*)
Albano, E.L. *et al, Chem. Comm.*, 1968, 357 (*2-Ac, pmr*)
Albano, E.L. *et al, Carbohydr. Res.*, 1969, **9**, 149 (*2-Ac, ir*)
Jacobsen, S. *et al, Acta Chem. Scand., Ser. B*, 1974, **28**, 1024 (*2-benzoyl*)

6-Bromo-6-deoxyaltrose B-1-00249



α-D-Pyranose-*form*

$C_6H_{11}BrO_5$ M 243.0

D-form

3,4-Di-Me, 2,5-dibenzyl: [126215-06-3]. $C_{22}H_{27}BrO_5$ M 451.3 Syrup.

α-D-Pyranose-form

Me glycoside: $C_7H_{13}BrO_5$ M 257.0 Syrup. $[\alpha]_D$ +80 (H_2O).

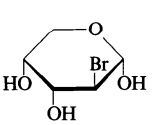
Me glycoside, 2,4-dibenzoyl, 3-Ac: [120123-45-7]. $C_{23}H_{23}BrO_8$ M 507.3 Syrup. $[\alpha]_D$ −24.2 (c, 1.0 in $CHCl_3$).

Me glycoside, 4-benzoyl, 2,3-di-Ac: [73139-31-8]. $C_{18}H_{21}BrO_8$ M 445.2 Cryst. Mp 112-114°. $[\alpha]_D$ +48 ($CHCl_3$).

Me glycoside, 2,3,4-tribenzoyl: $C_{28}H_{25}BrO_8$ M 569.4 Cryst. Mp 146-147°. $[\alpha]_D$ 0 ($CHCl_3$).

Rosenfeld, D.A. *et al, J.A.C.S.*, 1948, **70**, 2204 (*Me gly*)
Chana, J.S. *et al, Chem. Comm.*, 1988, 94 (*di-Ac, pmr*)
Aqeel, A. *et al, J. Carbohydr. Chem.*, 1989, **8**, 405 (*3-Ac, pmr*)

2-Bromo-2-deoxyarabinose B-1-00250



α-D-Pyranose-*form*

$C_5H_9BrO_4$ M 213.0

D-form

Cryst. Mp 125°. $[\alpha]_D$ −121 (H_2O).

α-D-Pyranose-form

1-Benzoyl, 3,4-di-Ac: [50271-27-7]. $C_{16}H_{17}BrO_7$ M 401.2 Cryst. (Et_2O/pentane). Mp 144-145°. $[\alpha]_D^{20}$ −5.57 (c, 2.3 in $CHCl_3$).

Me glycoside: Methyl 2-bromo-2-deoxy-α-D-arabinopyranoside $C_6H_{11}BrO_4$ M 227.0 Cryst. Mp 91-92°. $[\alpha]_D$ −68 (MeOH).

α-D-Furanose-form

Me glycoside, 3,5-di-Ac: [23259-82-7]. $C_{10}H_{15}BrO_6$ M 311.1 Oil.

β-D-Furanose-form

Me glycoside, 3,5-di-Ac: [55734-55-9]. Cryst. (Et_2O/pentane). Mp 80-81°. $[\alpha]_D^{21}$ −107 (c, 2.5 in $CHCl_3$).

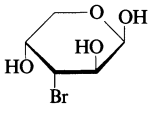
Me glycoside, 3,5-dibenzoyl: [55734-50-4]. $C_{20}H_{19}BrO_6$ M 435.2 Cryst. (Et_2O/pentane). Mp 109-109.5°. $[\alpha]_D^{20}$ −98.6 (c, 2.7 in $CHCl_3$).

L-form

Cryst. Mp 122°. $[\alpha]_D$ +116 (H_2O).

Kent, P.W. *et al, J.C.S.*, 1964, 6196 (*synth*, D-form, L-form, α-Me pyr)
Reist, E.J. *et al, Carbohydr. Res.*, 1969, **9**, 71 (α-D-fur di-Ac, ir, pmr)
Bock, K. *et al, J.C.S. Perkin 1*, 1973, 1456 (*α-Me pyr*)
Bock, K. *et al, Acta Chem. Scand., Ser. B*, 1975, **29**, 185 (*β*-D-fur derivs, pmr)

3-Bromo-3-deoxyarabinose B-1-00251



β-D-Pyranose-*form*

$C_5H_9BrO_4$ M 213.0

β-D-Pyranose-form

Me glycoside: $C_6H_{11}BrO_4$ M 227.0 Syrup.

Me glycoside, 2,4-dibenzoyl: [54621-51-1]. $C_{20}H_{19}BrO_6$ M 435.2 Cryst. (cyclohexane). Mp 82-86°. $[\alpha]_D^{25}$ −267.8 (c, 1.0 in $CHCl_3$).

α-D-Furanose-form

Me glycoside, 5-Ac: [13052-00-1]. $C_8H_{13}BrO_5$ M 269.0 Syrup.

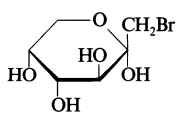
β-D-Furanose-form

Me glycoside, 5-Ac: [13051-99-5]. Oil. $[\alpha]_D^{22}$ −89 (c, 0.91 in $CHCl_3$).

Me glycoside, 5-benozyl: [43168-74-7]. $C_{13}H_{15}BrO_5$ M 331.1 Syrup. $[\alpha]_D$ −73 (c, 1.1 in $CHCl_3$).

Reist, E.J. *et al, Methods Carbohydr. Chem.*, 1972, **6**, 179 (*5-Ac, pmr*)
Ritchie, R.G.S., *Chem. Ind. (London)*, 1973, 530 (*5-benzoyl*)
Jacobsen, S. *et al, Acta Chem. Scand., Ser. B*, 1974, **28**, 866 (*β-Me pyr deriv, pmr*)

1-Bromo-1-deoxyfructose B-1-00252



α-D-Pyranose-*form*

$C_6H_{11}BrO_5$ M 243.0

D-form

Phenylosazone: Cryst. (EtOH). Mp 202-205°.

Tetra-Ac: $C_{14}H_{19}BrO_9$ M 411.2 Cryst. Mp 68°. $[\alpha]_D$ +62.5 ($CHCl_3$).

α-D-Pyranose-form

Me glycoside: [119645-60-2]. *Methyl 1-bromo-1-deoxy-α-D-fructopyranoside* $C_7H_{13}BrO_5$ M 257.0 Cryst. Mp 84-85°. $[\alpha]_D^{25}$ −4.3 (c, 0.16 in H_2O).

β-D-Pyranose-form

2,3:4,5-Di-O-isopropylidene: [10225-89-5]. $C_{12}H_{19}BrO_5$ M 323.1 Cryst. (Et_2O/petrol). Mp 46-47°. $[\alpha]_D^{23}$ −34.4 (c, 0.48 in $CHCl_3$).

Me glycoside: [119645-61-3]. *Methyl 1-bromo-1-deoxy-β-D-fructopyranoside* $C_7H_{13}BrO_5$ M 257.0 Cryst. Mp 86-87°. $[\alpha]_D^{25}$ −126.9 (c, 0.13 in H_2O).

β-D-Furanose-form

2,3-O-Isopropylidene, 6-benzoyl: [83032-01-3]. $C_{16}H_{19}BrO_6$ M 387.2 Cryst. (MeOH). Mp 89-90°. $[\alpha]_D^{25}$ +13.9 ($CHCl_3$).

L-form

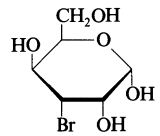
Tetra-Ac: [23261-11-2]. Cryst. (Et_2O/petrol). Mp 66-67°. $[\alpha]_D^{23}$ −65 (c, 4.0 in $CHCl_3$).

DL-form

Tetra-Ac: [23261-12-3]. Cryst. (Et_2O/petrol). Mp 92°. $[\alpha]_D^{23}$ 0 (c, 0.4 in $CHCl_3$).

Wolfrom, M.L. *et al, J.A.C.S.*, 1942, **64**, 1701 (D-tetra-Ac)
Humphlett, W.J., *Carbohydr. Res.*, 1968, **7**, 431 (L-tetra-Ac, DL-tetra-Ac)
Barnett, J.E.G. *et al, Carbohydr. Res.*, 1972, **25**, 511 (*diisopropylidene*)
Guthrie, R.D. *et al, Aust. J. Chem.*, 1982, **35**, 1003 (*β*-D-fur deriv, pmr)
Sinclair, H.B., *Carbohydr. Res.*, 1988, **181**, 115 (*α-Me pyr, β-Me pyr, cmr*)

3-Bromo-3-deoxygulose B-1-00253



α-D-Pyranose-*form*

$C_6H_{11}BrO_5$ M 243.0

α-D-Pyranose-form

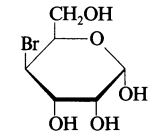
Me glycoside, 4,6-O-benzylidene, 2-Ac: $C_{16}H_{19}BrO_6$ M 387.2 Cryst. Mp 128-129°. $[\alpha]_D$ +67.5 ($CHCl_3$).

β-D-Pyranose-form

Me glycoside, 6-benzoyl: [24921-01-5]. $C_{14}H_{17}BrO_6$ M 361.1 Syrup. $[\alpha]_D^{25}$ −6 (c, 1.65 in $CHCl_3$).

Hedgley, E.J. *et al, J.C.S.*, 1963, 4701 (*α-Me pyr deriv*)
Hanessian, S. *et al, J.O.C.*, 1969, **34**, 1035 (*β-Me pyr deriv*)

4-Bromo-4-deoxygulose B-1-00254



α-D-Pyranose-*form*

$C_6H_{11}BrO_5$ M 243.0

α-D-Pyranose-form

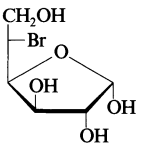
Me glycoside, 2,3-bis(3,5-dinitrobenzoyl), 6-[dimethyl(1,1,2-trimethylpropyl)silyl]: [128843-93-6].
Mp 110-114°. $[\alpha]_D^{25}$ +75.4 (c, 0.8 in $CHCl_3$).

Me glycoside, 2,3-anhydro, 6-trityl: [118360-83-1].
$C_{26}H_{25}BrO_4$ M 481.3 $[\alpha]_D^{31}$ −31 (c, 0.99 in $CHCl_3$).

Tatsuta, H. *et al, Bull. Chem. Soc. Jpn.*, 1988, **61**, 2525 (*anhydro, pmr*)

Rehnberg, N. *et al, J.O.C.*, 1990, **55**, 5467 (*silyl, pmr, cmr*)

5-Bromo-5-deoxyidose B-1-00255



$C_6H_{11}BrO_5$ M 243.0

β-L-Furanose-form

1,2-O-Isopropylidene: [130619-43-1].
$C_9H_{15}BrO_5$ M 283.1 Syrup. $[\alpha]_D^{20}$ −6.1 (c, 3.0 in $CHCl_3$).

1,2-O-Isopropylidene, 6-Me, 3-benzoyl: [18930-14-8].
$C_{17}H_{21}BrO_6$ M 401.2 Syrup. $[\alpha]_D^{25}$ +4.7 (c, 4.15 in $CHCl_3$).

1,2-O-Isopropylidene, 6-(tetrahydro-2H-pyran-2-yl): [130619-45-3].
$C_{14}H_{23}BrO_6$ M 367.2 Syrup.

1,2;3,6-Di-O-isopropylidene: [82893-16-1].
$C_{12}H_{19}BrO_5$ M 323.1 Syrup. $[\alpha]_D^{22}$ +51.6 (c, 1.4 in $CHCl_3$).

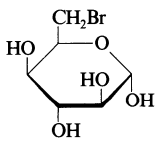
[130619-54-4]

Hanessian, S. *et al, J.O.C.*, 1969, **34**, 1053 (*6-Me, ir*)

Kunz, H. *et al, Annalen*, 1982, 1245 (*diisopropylidene*)

Dax, R. *et al, J. Carbohydr. Chem.*, 1990, **9**, 479 (*tetrahydropyranyl, pmr, cmr*)

6-Bromo-6-deoxyidose B-1-00256



α-D-Pyranose-*form*

$C_6H_{11}BrO_5$ M 243.0

α-D-Pyranose-form

Tetra-Ac: [29884-71-7].
$C_{14}H_{19}BrO_9$ M 411.2 Cryst. (EtOH). Mp 117-118°. $[\alpha]_D^{20}$ +58 (c, 2.5 in $CHCl_3$).

Me glycoside: [125280-08-2].
$C_7H_{13}BrO_5$ M 257.0 Cryst. (CH_2Cl_2/hexane). Mp 68.5-70°. $[\alpha]_D^{25}$ +85.1 ($CHCl_3$).

Me glycoside, 4-benzoyl: [125237-71-0].
$C_{14}H_{17}BrO_6$ M 361.1 Cryst. (CH_2Cl_2/hexane). Mp 106.5-107.5°. $[\alpha]_D^{28}$ +104.1 ($CHCl_3$).

Me glycoside, tribenzoyl: [79635-97-5].
Cryst. (EtOH). Mp 165-166°.

β-D-Furanose-form

1,2-O-Isopropylidene, 3,5-dibenzoyl: [108802-08-0].
$C_{23}H_{23}BrO_7$ M 491.3 Syrup. $[\alpha]_D$ −6 (c, 0.45 in $CHCl_3$).

β-L-Furanose-form

1,2-O-Isopropylidene, 5-benzoyl: [33999-40-5].
$C_{16}H_{19}BrO_6$ M 387.2 Syrup.
Attempted crystallisation led to dec.

1,2-O-Isopropylidene, 5-benzoyl, 3-Ac: [34010-38-3].
$C_{18}H_{21}BrO_7$ M 429.2 Syrup. $[\alpha]_D^{25}$ −8 (c, 4 in $CHCl_3$).

1,2-O-Isopropylidene, 3,5-dibenzyl: [87357-55-9].
$C_{23}H_{27}BrO_5$ M 463.3 Cryst. Mp 131-134°. $[\alpha]_D^{22}$ −20.73 (c, 0.5 in $CHCl_3$).

Paulsen, H. *et al, Chem. Ber.*, 1970, **103**, 2450 (*tetra-Ac*)

Chalk, R.C. *et al, Carbohydr. Res.*, 1971, **20**, 151 (*β-L-fur deriv, pmr*)

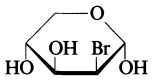
Neeser, J.R. *et al, Helv. Chim. Acta*, 1983, **66**, 1018 (*β-L-fur deriv, pmr*)

Jacobsen, S., *Acta Chem. Scand., Ser. B*, 1984, **38**, 157 (*Me pyr tribenzoyl*)

Guiliano, R.M. *et al, Carbohydr. Res.*, 1989, **191**, 1 (*Me α-D-pyr deriv*)

Lee, C.K., *Carbohydr. Res.*, 1990, **205**, 203 (*β-D-fur deriv*)

2-Bromo-2-deoxylyxose B-1-00257



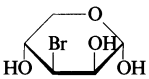
$C_5H_9BrO_4$ M 213.0

α-D-Pyranose-form

Me glycoside, di-Ac: [51385-05-8].
$C_{10}H_{15}BrO_6$ M 311.1 Mp 56-57°. $[\alpha]_D^{25}$ −7 (c, 1.49 in $CHCl_3$).

Van Es, T., *J. S. Afr. Chem. Inst.*, 1973, **26**, 152 (*di-Ac, pmr*)

3-Bromo-3-deoxylyxose B-1-00258



α-D-Pyranose-*form*

$C_5H_9BrO_4$ M 213.0

α-D-Pyranose-form

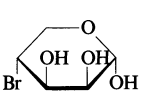
Me glycoside, dibenzoyl: [54621-50-0].
$C_{20}H_{19}BrO_6$ M 435.2 Cryst. (Et_2O/pentane). Mp 103-105°. $[\alpha]_D^{25}$ −125.4 (c, 1.3 in $CHCl_3$).

β-D-Pyranose-form

Me glycoside, 4-benzoyl, 2-Me: [54621-61-3].
$C_{14}H_{17}BrO_5$ M 345.1 Syrup. $[\alpha]_D^{21}$ −33.7 (c, 1.3 in $CHCl_3$).

Jacobsen, S. *et al, Acta Chem. Scand., Ser. B*, 1974, **28**, 866 (*Me gly deriv, pmr*)

4-Bromo-4-deoxylyxose B-1-00259



α-D-Pyranose-*form*

$C_5H_9BrO_4$ M 213.0

D-Pyranose-form

Me glycoside:
$C_6H_{11}BrO_4$ M 227.0 Cryst. Mp 134-135°. $[\alpha]_D$ +14.6 (MeOH).

α-D-Pyranose-form

Benzyl glycoside: [104292-63-9].
$C_{12}H_{15}BrO_4$ M 303.1 Cryst. (toluene). Mp 139-142°. $[\alpha]_D^{23}$ −62 (c, 0.8 in $CDCl_3$).

α-L-Pyranose-form

1-Benzoyl, 2,3-di-Ac:
$C_{16}H_{17}BrO_7$ M 401.2 Cryst. (Et_2O/pentane). Mp 149-150°. $[\alpha]_D^{20}$ −60.5 (c, 1.0 in $CHCl_3$).

Benzyl glycoside: [104292-62-8].
Cryst. (toluene). Mp 139-141°. $[\alpha]_D^{23}$ −61 (c, 0.9 in $CDCl_3$).

Benzyl glycoside, 2,3-O-isopropylidene: [123836-17-9].
$C_{15}H_{19}BrO_4$ M 343.2 Syrup.

Me glycoside, 2,3-anhydro: [106966-39-6].
$C_6H_9BrO_3$ M 209.0 Syrup. Bp_1 85°. $[\alpha]_D^{20}$ −68 (c, 0.37 in $CHCl_3$).

β-L-Pyranose-form

Benzyl glycoside: [112348-36-4].
Cryst. (EtOH). Mp 55-56°. $[\alpha]_D^{25}$ −72 (c, 0.47 in $CHCl_3$).

Benzyl glycoside, 2-benzoyl: [112348-34-2].
$C_{19}H_{19}BrO_5$ M 407.2 Syrup. $[\alpha]_D^{25}$ +103 (c, 0.68 in $CHCl_3$).

Benzyl glycoside, dibenzoyl: [112348-35-3].
$C_{26}H_{23}BrO_6$ M 511.3 Solid. $[\alpha]_D$ +118 (c, 0.94 in $CHCl_3$).

Benzyl glycoside, 2,3-O-isopropylidene: [123836-23-7].
Syrup.

Kent, P.W. *et al, J.C.S.*, 1953, 416 (*Me pyranoside*)

Bock, K. *et al, J.C.S. Perkin 1*, 1973, 1456 (*α-L-pyr deriv, ir, pmr*)

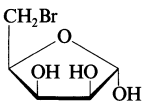
Canet, G. *et al, Carbohydr. Res.*, 1986, **152**, 292 (*α-L-Me gly, ir, pmr*)

Sundin, A. *et al, J.O.C.*, 1986, **51**, 3927 (*α-L-benzyl gly, α-D-benzyl gly, pmr, cmr*)

Rao, M.V. *et al, J.O.C.*, 1988, **53**, 1432, 1184 (*β-L-benzyl gly*)

Keck, G.E. *et al, J.O.C.*, 1990, **54**, 5845 (*benzyl gly isopropylidene*)

5-Bromo-5-deoxylyxose B-1-00260



α-D-Furanose-*form*

$C_5H_9BrO_4$ M 213.0

D-form [42854-92-2]
Syrup.

2,3-O-Isopropylidene: [121668-05-1].
$C_8H_{13}BrO_4$ M 253.0 Syrup.

α-D-furanose-form

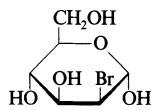
Benzyl glycoside, 2,3-O-isopropylidene: [42854-91-1].
$C_{15}H_{19}BrO_4$ M 343.2 Liq. $Bp_{0.03}$ 130°. $[\alpha]_D^{20}$ +91.6 (c, 1.31 in MeOH).

DL-form [36663-35-1]
Syrup.

Tamura, T. *et al, J.O.C.*, 1974, **39**, 38 (D-form, α-D-fur deriv, pmr)

Webb, T.H. *et al, Tet. Lett.*, 1988, **29**, 6823 (D-isopropylidene)

2-Bromo-2-deoxymannose B-1-00261



α-D-Pyranose-*form*

$C_6H_{11}BrO_5$ M 243.0

D-form

Solid. Mp 120°. $[\alpha]_D^{18}$ +2.72 (H_2O).

α-D-Pyranose-form

Tetra-Ac: [79733-39-4].
$C_{14}H_{19}BrO_9$ M 411.2 Syrup.

1-Benzoyl, 3,4,6-tri-Ac: [19237-69-5].
$C_{19}H_{21}BrO_9$ M 473.2 Cryst. Mp 168-169°. $[\alpha]_D^{28}$ +62.3 (c, 1.54 in $CHCl_3$).

Me glycoside: Methyl 2-bromo-2-deoxy-α-D-mannopyranoside
$C_7H_{13}BrO_5$ M 257.0 Syrup. $[\alpha]_D$ +47.5 ($CHCl_3$).

Me glycoside, tri-Ac: [63069-63-6].
$C_{13}H_{19}BrO_8$ M 383.1 Cryst. Mp 115-116°. $[\alpha]_D$ −92 (CCl_4).

Me glycoside, 4,6-O-benzylidene (R-)*:* [131564-60-8].
$C_{14}H_{17}BrO_5$ M 345.1 Cryst. (Et_2O/petrol). Mp 83-85° (77-78°). $[\alpha]_D$ +18 (c, 1.0 in $CHCl_3$).

Me glycoside, 4,6-O-benzylidene (R-)*, 3-Ac:* [131564-61-9].
$C_{16}H_{19}BrO_6$ M 387.2 Cryst. $[\alpha]_D$ +7.4 (c, 1.0 in CH_2Cl_2).

Me glycoside, tribenzyl: [77770-58-2].
$C_{28}H_{31}BrO_5$ M 527.4 Syrup. $[\alpha]_D^{22}$ +21 (c, 1.0 in $CHCl_3$).

β-D-Pyranose-form

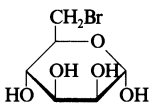
Me glycoside: Methyl 2-bromo-2-deoxy-β-D-mannopyranoside
$C_7H_{13}BrO_5$ M 257.0 Cryst. Mp 181-182°. $[\alpha]_D$ −64 (H_2O).

Me glycoside, tri-Ac: Cryst. Mp 115-116°. $[\alpha]_D$ −92 (CCl_4).

Me glycoside, tribenzyl: Syrup. $[\alpha]_D^{22}$ −43 (c, 1.25 in $CHCl_3$).

Manolopoulos, P.T. *et al, J.A.C.S.*, 1962, **84**, 2203 (*β-Me gly*)
Kent, P.W. *et al, J.C.S.*, 1963, 3273; 1964, 6196 (D-form, α-Me gly, α-Me gly benzylidene)
Gross, P.H. *et al, Annalen*, 1965, **681**, 225 (*α-Me gly*)
Hall, L.D. *et al, Chem. Comm.*, 1968, 35 (*benzoyl, tri-Ac*)
Classen, B., *Can. J. Chem.*, 1981, **59**, 339 (*α-Me gly tribenzyl, β-Me gly tribenzyl*)
Binkley, R.W. *et al, J. Carbohydr. Chem.*, 1987, **6**, 203 (*tetra-Ac, pmr, cmr*)
Khan, R. *et al, Carbohydr. Res.*, 1990, **205**, 211 (*α-Me gly benzylidene, pmr, cmr, ms*)

6-Bromo-6-deoxymannose B-1-00262



$C_6H_{11}BrO_5$ M 243.0

α-D-Pyranose-form

Me glycoside: [52340-56-4].
$C_7H_{13}BrO_5$ M 257.0 Cryst. Mp 97-99°. $[\alpha]_D^{20}$ +57 (c, 1.5 in H_2O).

Me glycoside, tri-Ac: [30589-67-4].
$C_{13}H_{19}BrO_8$ M 383.1 Cryst. (cyclohexane). Mp 78-81°. $[\alpha]_D^{20}$ +53 (c, 0.1 in $CHCl_3$).

Me glycoside, 4-benzoyl: [18929-78-7].
$C_{14}H_{17}BrO_6$ M 361.1 Amorph. solid (Et_2O/pentane). $[\alpha]_D^{25}$ −124 (c, 2.39 in $CHCl_3$).

Me glycoside, 4-benzoyl, 2,3-di-Ac: [18929-80-1].
$C_{18}H_{21}BrO_8$ M 445.2 Cryst. (Et_2O/petrol). Mp 120-121°. $[\alpha]_D^{25}$ +21 (c, 1.09 in $CHCl_3$).

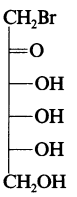
Me glycoside, 2,3-dibenzoyl: [135216-49-8].
$C_{21}H_{21}BrO_7$ M 465.2 Cryst. (EtOH). Mp 182-184°. $[\alpha]_D^{20}$ −120 ($CHCl_3$).

Me glycoside, 2,3-dibenzoyl, 4-tosyl: [135216-50-1].
$C_{28}H_{27}BrO_9S$ M 619.4 Cryst. (EtOH). Mp 109-110°. $[\alpha]_D^{20}$ −116 ($CHCl_3$).

Me glycoside, tribenzoyl: [18929-79-8].
$C_{28}H_{25}BrO_8$ M 569.4 Cryst. Mp 180-181°. $[\alpha]_D^{25}$ −115 (c, 0.4 in $CHCl_3$).

Levene, P.A. *et al, Coll. Czech. Chem. Comm.*, 1934, **6**, 354 (*Me gly*)
Horton, D. *et al, Carbohydr. Res.*, 1968, **7**, 101 (*tri-Ac*)
Hanessian, S. *et al, J.O.C.*, 1969, **34**, 1035 (*Me gly deriv*)
Shulman, M.L. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1973, 414; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1973, 394 (*tri-Ac*)
Cicero, D. *et al, Carbohydr. Res.*, 1991, **211**, 295 (*Me gly deriv*)

1-Bromo-1-deoxypsicose B-1-00263



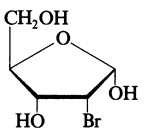
$C_6H_{11}BrO_5$ M 243.0

D-form

Tetra-Ac: [51296-43-6].
$C_{14}H_{19}BrO_9$ M 411.2 Cryst. Mp 77-79°. $[\alpha]_D$ −15.1 ($CHCl_3$).

Wolfrom, M.L. *et al, J.A.C.S.*, 1945, **67**, 1793 (*tetra-Ac*)
Vanek, T. *et al, Nucleic Acids Res., Spec. Publ.*, 1978, **4**, 173; *CA*, **90**, 87812w (*tetra-Ac*)

2-Bromo-2-deoxyribose B-1-00264



α-D-Furanose-*form*

$C_5H_9BrO_4$ M 213.0

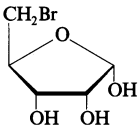
α-D-Furanose-form

Me glycoside, dibenzoyl: [55734-54-8].
$C_{20}H_{19}BrO_6$ M 435.2 Syrup.

β-D-Furanose-form [125155-49-9]
Syrup.

Bock, K. *et al, Acta Chem. Scand., Ser. B*, 1975, **29**, 185 (*α-fur deriv, pmr*)
Ilicheva, I.A. *et al, Bioorg. Khim.*, 1989, **15**, 800; *Sov. J. Bioorg. Chem. (Engl. Transl.)*, 1989, **15**, 428 (*β-fur*)

5-Bromo-5-deoxyribose B-1-00265



α-D-Furanose-*form*

$C_5H_9BrO_4$ M 213.0

α-D-Furanose-form

Me glycoside, 2,3-O-isopropylidene: [120142-51-0].
$C_9H_{15}BrO_4$ M 267.1 Syrup.

β-D-Furanose-form

2,3-Dibenzoyl, 1-Ac: [120033-32-1].
$C_{21}H_{19}BrO_7$ M 463.2 Cryst. (hexane). Mp 68.6-69°.

Me glycoside, 2,3-dibenzoyl: [120033-28-5].
$C_{20}H_{19}BrO_6$ M 435.2 Cryst. (hexane). Mp 60-61°.

Me glycoside, 2,3-O-isopropylidene: [38838-05-0].
Syrup. $Bp_{0.1}$ 72°. $[\alpha]_D^{25}$ −80 (c, 2.61 in $CHCl_3$).

β-L-Furanose-form

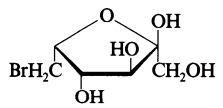
Me glycoside, 2,3-O-isopropylidene: [118244-91-0].
Liq. $[\alpha]_D^{25}$ +65 (c, 1.0 in $CHCl_3$).

β-DL-Furanose-form

Me glycoside, 2,3-O-isopropylidene: [118244-92-1].
Liq.

Hanessian, S. *et al, Carbohydr. Res.*, 1972, **24**, 45 (*β-Me gly deriv*)
Kiss, J. *et al, Helv. Chim. Acta*, 1982, **65**, 1522 (*Me gly deriv*)
Wagner, J. *et al, Helv. Chim. Acta*, 1988, **71**, 624 (*β-L-fur deriv, β-DL-fur deriv*)
Raju, N. *et al, J. Med. Chem.*, 1989, **32**, 1307 (*α-fur deriv, β-fur deriv*)

6-Bromo-6-deoxysorbose B-1-00266



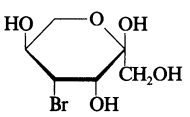
$C_6H_{11}BrO_5$ M 243.0

α-L-Furanose-form

2,3-O-Isopropylidene: [121564-08-7].
$C_9H_{15}BrO_5$ M 283.1 Mp 109-110°. $[\alpha]_D^{20}$ +13.6 (c, 1.0 in MeOH).

Beaupere, D. *et al, J. Carbohydr. Chem.*, 1989, **8**, 159 (*isopropylidene, pmr, cmr*)

4-Bromo-4-deoxytagatose B-1-00267



α-L-Pyranose-*form*

$C_6H_{11}BrO_5$ M 243.0

α-L-Pyranose-form

Me glycoside, tri-Ac: [19877-24-8].
$C_{13}H_{19}BrO_8$ M 383.1 Cryst. (Et_2O/petrol). Mp 136-138°. $[\alpha]_D^{22}$ −30.9 (c, 1.05 in $CHCl_3$).

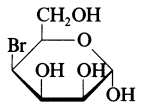
β-Pyranose-form

Me glycoside, tri-Ac: [19877-75-9].

Syrup. $[\alpha]_D^{23}$ +51.3 (c, 0.83 in $CHCl_3$).

Katsuhara, M. *et al, Bull. Chem. Soc. Jpn.*, 1968, **41**, 1208 (*tri-Ac, pmr*)

4-Bromo-4-deoxytalose B-1-00268



α-D-Pyranose-*form*

$C_6H_{11}BrO_5$ M 243.0

α-D-Pyranose-form

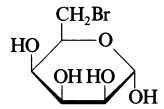
Me glycoside: [77770-63-9].
$C_7H_{13}BrO_5$ M 257.0 Cryst. (EtOAc/petrol). Mp 105°. $[\alpha]_D^{22}$ +102 (c, 1.0 in H_2O).

Me glycoside, tri-Ac: [77770-65-1].
$C_{13}H_{19}BrO_8$ M 383.1 Syrup.

Me glycoside, 6-trityl: [77770-64-0].
$C_{26}H_{27}BrO_5$ M 499.4 Syrup.

Classon, B. *et al, Can. J. Chem.*, 1981, **59**, 339 (*α-Me gly deriv*)

6-Bromo-6-deoxytalose B-1-00269



$C_6H_{11}BrO_5$ M 243.0

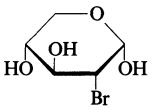
α-D-Pyranose-form

Me glycoside, 2,3-anhydro, 4-benzoyl: [18929-81-2].
$C_{14}H_{15}BrO_5$ M 343.1 Cryst. (Et_2O/pentane). Mp 134-135°. $[\alpha]_D^{25}$ −64 (c, 0.3 in $CHCl_3$).

Hanessian, S. *et al, J.O.C.*, 1969, **34**, 1035 (*Me gly deriv, ir*)

Hanessian, S. *et al, Methods Carbohydr. Chem.*, 1972, **6**, 183 (*Me gly deriv*)

2-Bromo-2-deoxyxylose B-1-00270



α-D-Pyranose-*form*

$C_5H_9BrO_4$ M 213.0

D-form

3,4-Dibenzoyl: [50271-31-3].
$C_{19}H_{17}BrO_6$ M 421.2 Cryst. (Et_2O/pentane). Mp 145-146°. $[\alpha]_D^{20}$ −64.5 → −30.8 (equilib.) (c, 2.5 in $CHCl_3$).

α-D-Pyranose-form

Tribenzoyl: [50271-36-8].
$C_{26}H_{21}BrO_7$ M 525.3 Syrup.

β-D-Pyranose-form

1-Benzoyl, 3,4-di-Ac: [50271-22-2].
$C_{16}H_{17}BrO_7$ M 401.2 Cryst. (Et_2O/pentane). Mp 120-121°. $[\alpha]_D^{20}$ −25 (c, 1.8 in $CHCl_3$).

1,3-Dibenzoyl, 4-Ac: [50271-41-5].
$C_{21}H_{19}BrO_7$ M 463.2 Cryst. (Et_2O/pentane). Mp 65-68°. $[\alpha]_D^{21}$ +20.5 (c, 0.66 in $CHCl_3$).

α-D-Furanose-form

Me glycoside, di-Ac: [55734-58-2].
$C_{10}H_{15}BrO_6$ M 311.1 Syrup.

Me glycoside, dibenzoyl: [55734-56-0].
$C_{20}H_{19}BrO_6$ M 435.2 Syrup. $[\alpha]_D^{21}$ +163.1 (c, 5.9 in $CHCl_3$).

β-D-Furanose-form

Me glycoside, 5-Ac: [13051-98-4].
$C_8H_{13}BrO_5$ M 269.0 Oil. $[\alpha]_D^{22}$ −35 (c, 0.97 in $CHCl_3$).

Me glycoside, di-Ac: [55734-59-3].
Syrup.

Me glycoside, 3-benzoyl: [43168-70-3].
$C_{13}H_{15}BrO_5$ M 331.1 Syrup. $[\alpha]_D$ +29 (c, 3.3 in CCl_4).

Me glycoside, 5-benzoyl: [43168-69-0].
$C_{13}H_{15}BrO_5$ M 331.1 Syrup. $[\alpha]_D$ −16.6 (c, 4.7 in CCl_4).

Me glycoside, dibenzoyl: [43168-71-4].
Cryst. (MeOH). Mp 67.5-68°. $[\alpha]_D$ −6 (c, 1.06 in $CHCl_3$).

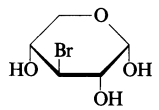
Reist, E.J. *et al, Methods Carbohydr. Chem.*, 1972, **6**, 179 (*β-Me fur Ac, uv, pmr*)

Ritchie, R.G.S. *et al, Chem. Ind. (London)*, 1973, 530 (*β-Me fur*)

Bock, K. *et al, J.C.S. Perkin 1*, 1973, 1456 (*α-pyr, β-pyr*)

Bock, K. *et al, Acta Chem. Scand., Ser. B*, 1975, **29**, 185 (D-form, α-Me fur)

3-Bromo-3-deoxyxylose B-1-00271



α-D-Pyranose-*form*

$C_5H_9BrO_4$ M 213.0

α-D-Pyranose-form

Benzyl glycoside, dibenzoyl: [112483-00-8].
$C_{26}H_{23}BrO_6$ M 511.3 Syrup.

β-D-Pyranose-form

Me glycoside:
$C_6H_{11}BrO_4$ M 227.0 Cryst. Mp 101-102°. $[\alpha]_D$ −16.4 (MeOH).

Benzyl glycoside, 2-Me: [128843-90-3].
$C_{13}H_{17}BrO_4$ M 317.1 Syrup.

Benzyl glycoside, 4-Me: [128843-91-4].
$C_{13}H_{17}BrO_4$ M 317.1 Cryst. (EtOAc/heptane). Mp 103-104°. $[\alpha]_D^{25}$ −39 (c, 1.7 in $CHCl_3$).

α-D-Furanose-form

Me glycoside, di-Ac: [23259-83-8].
$C_{10}H_{15}BrO_6$ M 311.1 Oil.

Me glycoside, dibenzoyl: [54621-63-5].
$C_{20}H_{19}BrO_6$ M 435.2 Syrup.

β-D-Furanose-form

Me glycoside, di-Ac: [23259-86-1].
Oil.

Me glycoside, dibenzoyl: [54621-64-6].
Syrup. $[\alpha]_D^{21}$ +31.8 (c, 3.0 in $CHCl_3$).

[112483-17-7]

Kent, P.W. *et al, J.C.S.*, 1949, 1232 (*β-Me pyr*)

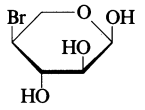
Reist, E.J. *et al, Carbohydr. Res.*, 1969, **9**, 71 (*Me gly di-Ac, pmr, ir*)

Jacobsen, S. *et al, Acta Chem. Scand., Ser. B*, 1974, **28**, 866 (*Me gly dibenzoyl*)

Rao, M.V. *et al, J.O.C.*, 1988, **53**, 1184 (*α-benzyl gly*)

Rehnberg, N. *et al, J.O.C.*, 1990, **55**, 5467 (*β-benzyl gly, pmr*)

4-Bromo-4-deoxyxylose B-1-00272



α-L-Pyranose-*form*

$C_5H_9BrO_4$ M 213.0

α-L-Pyranose-form

1,2-O-Benzylidene: [55169-80-7].
$C_{12}H_{13}BrO_4$ M 301.1 Mp 125-126°. $[\alpha]_D^{21}$ −43.3 (c, 1.7 in $CHCl_3$).

Me glycoside, dibenzoyl: [18930-05-7].
$C_{20}H_{19}BrO_6$ M 435.2 Cryst. (cyclohexane). Mp 109-110°. $[\alpha]_D^{25}$ −129.7 (c, 1.1 in $CHCl_3$).

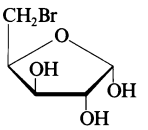
Me glycoside, 3-benzoyl, 2-Me: [54621-62-4].
$C_{14}H_{17}BrO_5$ M 345.1 Cryst. (Et_2O/pentane). Mp 73-74°. $[\alpha]_D^{21}$ −76.2 (c, 1.3 in $CHCl_3$).

[55169-81-8]

Jacobsen, S. *et al, Acta Chem. Scand., Ser. B*, 1974, **28**, 866, 1024 (*benzylidene, α-Me gly deriv, pmr*)

Chana, J.S. *et al, Chem. Comm.*, 1988, 94 (*α-Me gly deriv*)

5-Bromo-5-deoxyxylose B-1-00273



α-D-Furanose-*form*

$C_5H_9BrO_4$ M 213.0

D-form [42854-95-5]
Syrup.

α-D-Furanose-form

1,2-O-Isopropylidene: [42854-94-4].
$C_8H_{13}BrO_4$ M 253.0 Needles (hexane). Mp 93-94°. $[\alpha]_D^{20}$ −22.2 (c, 1.58 in MeOH).

1,2-O-Isopropylidene, 3-benzoyl: [41164-25-4].
$C_{15}H_{17}BrO_5$ M 357.2 Glass. $[\alpha]_D^{25}$ −46.6 (c, 1.0 in $CHCl_3$).

1,2-O-Isopropylidene, 3-Me: [17954-93-7].
$C_9H_{15}BrO_4$ M 267.1 Syrup. $Bp_{0.2}$ 67°. $[\alpha]_D^{18}$ −77.6 (c, 1.0 in $CHCl_3$).

Me glycoside, di-Ac: [56570-73-1].
$C_{10}H_{15}BrO_6$ M 311.1 Syrup.

β-D-Furanose-form

Me glycoside, di-Ac: [56587-55-4].
Cryst.

DL-form [36663-36-2]
Syrup.

Inokawa, S. *et al, Bull. Chem. Soc. Jpn.*, 1968, **41**, 1472; 1973, **46**, 3301 (*3-Me*)

Culbertson, T.P. *et al, J.O.C.*, 1973, **38**, 3624 (*3-benzoyl, pmr*)

Tamura, T. *et al, J.O.C.*, 1974, **39**, 38 (*synth*, D-form, DL-form, isopropylidene, pmr, ir)

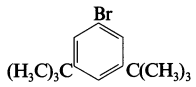
Hollenberg, D.H. *et al, Carbohydr. Res.*, 1975, **42**, 241 (*3-benzoyl, α-Me gly di-Ac, β-Me gly di-Ac, pmr*)

Pan, C. *et al, CA*, 1989, **110**, 8765p (*isopropylidene*)

1-Bromo-3,5-di-*tert*-butylbenzene B-1-00274

1-Bromo-3,5-bis(1,1-dimethylethyl)benzene

[22385-77-9]



$C_{14}H_{21}Br$ M 269.2
Cryst. (EtOH or hexane). Mp 64-64.5°. Bp_1 50-84°.

Bartlett, P.D. *et al*, *J.A.C.S.*, 1954, **76**, 2349.
Burgers, J. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1956, **75**, 1327 (*synth*)
de Konig, A.J., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1982, **101**, 385 (*pmr*)
Murphy, S. *et al*, *J.O.C.*, 1995, **60**, 2411 (*synth, pmr, cmr, ms*)

2-Bromo-1,3-di-*tert*-butylbenzene B-1-00275

2-Bromo-1,3-bis(1,1-dimethylethyl)benzene

[19715-32-3]

$C_{14}H_{21}Br$ M 269.2
Oil. $Bp_{0.1}$ 76-77°.

Rundel, W., *Chem. Ber.*, 1968, **101**, 2956 (*synth, ir, pmr*)
Yoshifuji, M. *et al*, *Tet. Lett.*, 1989, **30**, 5433 (*synth*)

2-Bromo-1,4-di-*tert*-butylbenzene B-1-00276

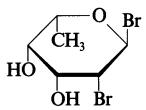
2-Bromo-1,4-bis(1,1-dimethylethyl)benzene

[6683-74-5]

$C_{14}H_{21}Br$ M 269.2
Oil. Bp_{12} 150°, $Bp_{0.4}$ 94-98°.

Theilacker, W. *et al*, *Chem. Ber.*, 1969, **102**, 2020 (*synth*)
Edler, R. *et al*, *Chem. Ber.*, 1989, **122**, 187 (*synth, ir, pmr*)

2-Bromo-2,6-dideoxytalopyranosyl bromide B-1-00277



$C_6H_{10}Br_2O_3$ M 289.9

α-L-form

Di-Ac: [103321-25-1].
$C_{10}H_{14}Br_2O_5$ M 374.0 Syrup. $[\alpha]_D^{22}$ −77 (c, 1.4 in CH_2Cl_2).

Horton, D. *et al*, *J.O.C.*, 1986, **51**, 3479 (*di-Ac, ms, cmr, pmr*)

4-Bromo-4,4-difluorobutanoic acid B-1-00278

[147345-36-6]

$BrCF_2CH_2CH_2COOH$

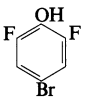
$C_4H_5BrF_2O_2$ M 202.9

Et ester:
$C_6H_9BrF_2O_2$ M 231.0 Oil. Bp_{25} 78-80°.

Hu, C. *et al*, *Chem. Comm.*, 1993, 72 (*synth, pmr, F-19 nmr, ir, ms*)

4-Bromo-2,6-difluorophenol B-1-00279

[104197-13-9]



$C_6H_3BrF_2O$ M 208.9
Oil.

Me ether: [104197-14-0]. *5-Bromo-1,3-difluoro-2-methoxybenzene. 4-Bromo-2,6-difluoroanisole*
$C_7H_5BrF_2O$ M 223.0 Bp_{15} 80-100°.

Kruse, L.L. *et al*, *Biochemistry*, 1986, 25, 7271 (*synth, pmr*)

3-Bromo-3,3-difluoropropene B-1-00280

[420-90-6]

$H_2C{=}CHCF_2Br$

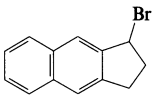
$C_3H_3BrF_2$ M 156.9
d 1.54. Bp 42°. n_D^{25} 1.3773.

Tarrant, P. *et al*, *J.A.C.S.*, 1955, **77**, 2783 (*synth*)

1-Bromo-2,3-dihydro-1*H*-benz[*f*]indene, 9CI B-1-00281

1-Bromobenz[f]indane

[146000-51-3]



$C_{13}H_{11}Br$ M 247.1

(±)-*form*
Yellow-brown solid (Et_2O/pentane). Mp 67-69°.

Josien, H. *et al*, *J. Med. Chem.*, 1994, **37**, 1586 (*synth, pmr*)

2-Bromo-3,3-dimethyl-1-butene, 9CI B-1-00282

[33693-77-5]

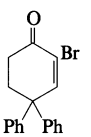
$(H_3C)_3CCBr{=}CH_2$

$C_6H_{11}Br$ M 163.0
Yellow liq. Bp_{100} 60°. n^{25} 1.457.

Pross, A. *et al*, *Aust. J. Chem.*, 1971, **24**, 1437 (*synth, ir, pmr*)
Kropp, P.J. *et al*, *J.O.C.*, 1994, **59**, 3102 (*synth, pmr*)

2-Bromo-4,4-diphenyl-2-cyclohexene-1-one, 9CI B-1-00283

[94331-87-0]

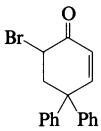


$C_{18}H_{15}BrO$ M 327.2
Cryst. (heptane). Mp 166.5-167.5°.

Bordwell, F.G. *et al*, *J.O.C.*, 1963, **28**, 2544 (*synth, ir*)
Malleron, J.-L. *et al*, *Synth. Commun.*, 1995, **25**, 2355 (*synth*)

6-Bromo-4,4-diphenyl-2-cyclohexen-1-one, 9CI B-1-00284

[33733-00-5]



$C_{18}H_{15}BrO$ M 327.2

(±)-*form*
Cryst. (hexane or EtOH). Mp 85-86°, Mp 108-112°.

Bordwell, F.G. *et al*, *J.O.C.*, 1963, **28**, 2544 (*synth, ir*)
Zimmerman, H.E. *et al*, *J.A.C.S.*, 1971, **93**, 3653 (*synth, ir, pmr*)
Matoba, K. *et al*, *Chem. Pharm. Bull.*, 1984, **32**, 4721 (*synth, pmr, ms*)

2-Bromodiphenyl ether B-1-00285

1-Bromo-2-phenoxybenzene, 9CI. o-*Bromophenyl phenyl ether, 8CI*

[7025-06-1]

$C_{12}H_9BrO$ M 249.1
Cryst. (MeOH). Mp 43.5-44.5°. $Bp_{0.1}$ 97-100°.

Sax, K.J. *et al*, *J.O.C.*, 1960, **25**, 1590 (*synth*)
Ames, D.E. *et al*, *Synthesis*, 1983, 234 (*synth*)

3-Bromodiphenyl ether B-1-00286

1-Bromo-3-phenoxybenzene, 9CI. m-*Bromophenyl phenyl ether, 8CI*

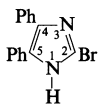
[6876-00-2]

$C_{12}H_9BrO$ M 249.1
Liq. Bp_{15} 168-171°, Bp_{10} 156-158°.

Gilman, H. *et al*, *J.O.C.*, 1960, **25**, 1194 (*synth*)
Sax, K.J. *et al*, *J.O.C.*, 1960, **25**, 1590 (*synth*)

2-Bromo-4,5-diphenyl-1*H*-imidazole, 9CI B-1-00287

[69045-24-5]



$C_{15}H_{11}BrN_2$ M 299.1
Solid (MeCN). Mp 153-155°.

Higley, C.A. *et al*, *J. Med. Chem.*, 1994, **37**, 3511 (*synth, pmr*)

2-Bromodiphenylmethane B-1-00288

1-Bromo-2-(phenylmethyl)benzene, 9CI. (o-*Bromophenyl)phenylmethane, 8CI. 1-Benzyl-2-bromobenzene*

[23450-18-2]

$C_{13}H_{11}Br$ M 247.1
Liq. $Bp_{21.5}$ 179-183°, Bp_{16} 166-167°, Bp_1 119-122°.

Vingiello, F.A. *et al, J.A.C.S.*, 1960, **25**, 2091 (*synth*)
Holt, P.F. *et al, J.C.S.*, 1961, 1405 (*synth*)
Barnes, I. *et al, J. Chem. Technol. Biotechnol.*, 1980, **30**, 731 (*synth*)

3-Bromodiphenylmethane B-1-00289

1-Bromo-3-(phenylmethyl)benzene, 9CI. (m-*Bromophenyl)phenylmethane, 8CI. 1-Benzyl-3-bromobenzene*

[27798-39-6]

$C_{13}H_{11}Br$ M 247.1
$Bp_{1.0}$ 129-130°. n_D^{20} 1.6056.

Holt, P.F. *et al, J.C.S.*, 1961, 1405 (*synth*)

2-Bromodiphenylmethanol B-1-00290

2-Bromo-α-phenylbenzenemethanol, 9CI. 2-Bromobenzhydrol, 8CI

[59142-47-1]

$C_{13}H_{11}BrO$ M 263.1

(+)-***form*** [143880-79-9]
Oil. $[\alpha]_D$ +46.6 (c, 1.3 in Me_2CO) (95% ee).

(±)-***form*** [137474-26-1]
Cryst. (petrol or C_6H_6/hexane). Mp 57-59°.

Me ether: [59142-71-1]. *1-Bromo-2-(methoxyphenylmethyl)benzene, 9CI*
$C_{14}H_{13}BrO$ M 277.1 Pale yellow liq. $Bp_{0.2}$ 125-128°.

[143880-86-8]

Koopal, S.A., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1915, **34**, 8, 158 (*synth*)
Bachmann, W.E. *et al, J.O.C.*, 1948, **13**, 916 (*synth*)
Martin, L.L. *et al, J. Med. Chem.*, 1976, **19**, 1315 (*synth*)
Brown, E. *et al, Tetrahedron: Asymmetry*, 1992, **3**, 841 (*synth, ir, pmr*)

3-Bromodiphenylmethanol B-1-00291

3-Bromo-α-phenylbenzenemethanol, 9CI. 3-Bromobenzhydrol, 8CI

[63012-04-4]

$C_{13}H_{11}BrO$ M 263.1

(+)-***form*** [123436-11-3]
Needles (petrol). Mp 56° (51-52°). $[\alpha]_D^{20}$ +33.8 (c, 2.5 in THF) (>95% ee).

(−)-***form*** [123436-15-7]
Needles (petrol). Mp 56° (51-52°). $[\alpha]_D^{20}$ −34.2 (c, 2.5 in THF) (>95% ee).

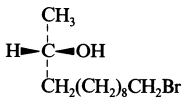
(±)-***form*** [137474-25-0]
Cryst. Mp 44°.

Ac:
$C_{15}H_{13}BrO_2$ M 305.1 $Bp_{0.3}$ 138-140°.

Bachmann, W.E. *et al, J.O.C.*, 1948, **13**, 916 (*synth*)
Puckowski, R.T. *et al, J.C.S.*, 1959, 3555 (*resoln*)
Wang, J.-T. *et al, Synthesis*, 1989, 291 (*synth, ir, pmr*)
Wang, J.-T. *et al, Chin. Chem. Lett.*, 1991, **2**, 349 (*synth*)
Toda, F. *et al, Tetrahedron: Asymmetry*, 1991, **2**, 873 (*resoln*)

12-Bromo-2-dodecanol B-1-00292

[141812-63-7]



$C_{12}H_{25}BrO$ M 265.2

(*S*)-***form***
Oil. $[\alpha]_D^{20}$ +2.6 (c, 0.6 in $CHCl_3$).

Baldwin, J.E. *et al, Tetrahedron*, 1992, **48**, 3413 (*synth, pmr, ir, ms*)
Enders, D. *et al, Annalen*, 1995, 1185 (*S-form, synth, ir, pmr, cmr, ms*)

(2-Bromoethyl) dimethylsulfonium(1+), 9CI B-1-00293

$BrCH_2CH_2S^{\oplus}Me_2$

$C_4H_{10}BrS^{\oplus}$ M 170.0 (ion)

Bromide: [28346-35-2]. *BES*
$C_4H_{10}Br_2S$ M 249.9 Cryst. (MeOH). Mp 146-147° dec.

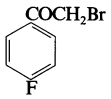
Iodide:
$C_4H_{10}BrIS$ M 296.9 Cryst. (MeOH). Mp 102° dec.

Doering, Wv.E. *et al, J.A.C.S.*, 1955, **77**, 514 (*synth*)

2-Bromo-4′-fluoroacetophenone B-1-00294

2-Bromo-1-(4-fluorophenyl)ethanone, 9CI. p-*Fluorophenacyl bromide. 1-(Bromoacetyl)-4-fluorobenzene*

[403-29-2]



C_8H_6BrFO M 217.0
Mp 48-50°. Bp_{12} 150°.

2,4-Dinitrophenylhydrazone: [7604-30-0]. Mp 212°.

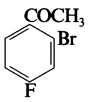
[112368-54-4]

Buu Hoi, N.-H. *et al, Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1949, **68**, 781 (*synth*)
Kitano, H. *et al, Kogyo Kagaku Zasshi*, 1955, **58**, 54; *CA*, **50**, 3293 (*synth*)
Henry, R.A. *et al, J.O.C.*, 1990, **55**, 1796 (*synth*)

2′-Bromo-4′-fluoroacetophenone, 8CI B-1-00295

1-(2-Bromo-4-fluorophenyl)ethanone, 9CI

[1006-39-9]



C_8H_6BrFO M 217.0
Bp_{10} 128-130°. n_D^{22} 1.5459.

Oxime:
C_8H_7BrFNO M 232.0 Cryst. (MeOH). Mp 104°.

Dinitrophenylhydrazone: Orange cryst. (AcOH). Mp 178°.
Thiosemicarbazide: Cryst. (EtOH). Mp 185°.

Quang, N.N. *et al, Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1964, 83, 1142 (*synth*)

5-Bromo-3-furancarboxaldehyde, 9CI B-1-00296

2-Bromo-4-formylfuran

[63387-54-2]

$C_5H_3BrO_2$ M 174.9
Oil. $Bp_{0.25}$ 55°.

Eur. Pat., 372 940, (1990); *CA*, **113**, 191137j (*synth, pmr*)

1-Bromo-1,1,2,2,3,3,-4,4,5,5,6,6,7,7,8,8,8-heptadecafluorooctane, 9CI B-1-00297

Perflubron, INN, USAN. *Perfluoroctyl bromide*

[423-55-2]

$F_3C(CF_2)_6CF_2Br$

C_8BrF_{17} M 498.9
Imaging agent for x-ray, ultrasound and pmr. Synthetic blood oxygen carrier. Bp 142°. Component of Oxygent and Imagent.

▶ LD_{50} (mus, ivn) 14720 mg/kg. RG8700000.

Haszeldine, R.N., *J.C.S.*, 1953, 3761 (*synth*)
U.S. Pat., 3 456 024, (1969) (*Dow Corning*); *CA*, **71**, 70078w (*synth*)
Lee, F.H. *et al, J. Pharm. Sci.*, 1978, **67**, 1038 (*metab*)
Patronas, N. *et al, Invest. Radiol.*, 1984, **19**, 570 (*use*)
Long, D.M. *et al, Biomater. Artif. Cells, Artif. Organs*, 1988, **16**, 411 (*rev*)
Freeman, D.M. *et al, Magn. Reson. Imaging*, 1988, **6**, 61 (*F-19 nmr*)
Andre, M. *et al, Invest. Radiol.*, 1990, **25**, 983 (*use*)
Mattrey, R.F. *et al, Biomater. Artif. Cells, Immobil. Biotech.*, 1992, **20**, 917; 1994, **22**, 1441, 1491, 1501 (*use*)
Biro, G.P., *Transfus. Med. Rev.*, 1993, **7**, 84 (*rev*)
Ohyanagi, H., *Artificial Red Cells*, (Ed., Tsuchida E.), J. Wiley, 1995, 199 (*rev*)

7-Bromoheptanal, 9CI B-1-00298

[54005-84-4]

$BrCH_2(CH_2)_5CHO$

$C_7H_{13}BrO$ M 193.0
Bp_1 95°, $Bp_{0.3}$ 80°.

Di-Me acetal: [130129-93-0]. *7-Bromo-1,1-dimethoxyheptane, 9CI*
$C_9H_{19}BrO_2$ M 239.1 Oil. $Bp_{1.7}$ 76-78°.

Kuwahara, S. *et al, Biosci., Biotechnol., Biochem.*, 1992, **56**, 1417 (*di-Me acetal*)
Bestmann, H.J. *et al, Synthesis*, 1993, 149 (*synth, pmr*)
Ballini, R. *et al, Helv. Chim. Acta*, 1995, **78**, 879 (*synth, pmr*)

7-Bromo-2-heptanone, 9CI B-1-00299

[50775-02-5]

$BrCH_2(CH_2)_4COCH_3$

$C_7H_{13}BrO$ M 193.0
Liq. Bp_{20} 118°, $Bp_{0.8}$ 68-70°. n_D^{20} 1.4707.

Semicarbazone: Mp 137°.

Minisci, F. *et al, Gazz. Chim. Ital.*, 1960, **90**, 1299 (*synth*)
Cuvigny, T. *et al, Annalen*, 1975, 719 (*synth, pmr, ir*)

Labadie, J.W. *et al*, *J.O.C.*, 1983, **48**, 4634 (*synth, pmr*)
Enders, D. *et al*, *Annalen*, 1995, 1173 (*synth*)

6-Bromohexanal, 9CI B-1-00300

[57978-00-4]

$BrCH_2(CH_2)_4CHO$

$C_6H_{11}BrO$ M 179.0
Bp_{14} 106-107°. n_D^{20} 1.4788.

2,4-Dinitrophenylhydrazone: [93715-86-7]. Mp 92-93°.

Brown, H.C. *et al*, *J.A.C.S.*, 1984, **106**, 8001 (*synth*)
Bestmann, H.J. *et al*, *Synthesis*, 1993, 149 (*synth, pmr*)

3-Bromo-6-hydroxy-2-methylpyridine B-1-00301

5-Bromo-6-methyl-2(1H)-pyridinone, 9CI

[54923-31-8]

C_6H_6BrNO M 188.0

NH-form

Needles (EtOH). Mp 204°.

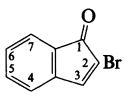
OH-form

Me ether: [126717-59-7]. *3-Bromo-6-methoxy-2-methylpyridine, 9CI*
C_7H_8BrNO M 202.0 Oil. Bp_6 95-96°.

Adams, R. *et al*, *J.A.C.S.*, 1949, **71**, 1186 (*synth*)
Shiao, M.-J. *et al*, *Heterocycles*, 1990, **31**, 819 (*Me ether*)
Langlois, Y. *et al*, *Synth. Commun.*, 1994, **24**, 1367 (*Me ether*)

2-Bromo-1*H*-inden-1-one, 9CI B-1-00302

[50870-60-5]



C_9H_5BrO M 209.0
Low melting brown-orange solid.

Boger, D.L. *et al*, *J.O.C.*, 1994, **59**, 3453 (*synth, pmr, cmr, ir*)

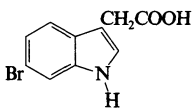
3-Bromo-1*H*-inden-1-one B-1-00303

[90271-93-5]

C_9H_5BrO M 209.0
Yellow needles. Mp 57.5-58°.

Straus, F. *et al*, *Ber.*, 1933, **66**, 1847 (*synth*)

6-Bromo-1*H*-indole-3-acetic acid B-1-00304



$C_{10}H_8BrNO_2$ M 254.0

Me ester: [152213-63-3]. *Methyl 6-bromo-1H-indole-3-acetate, 9CI*
$C_{11}H_{10}BrNO_2$ M 268.1 Alkaloid from the marine sponge *Pseudosuberites hyalinus*. Oil.

Amide: [152213-62-2]. *6-Bromo-1H-indole-3-acetamide, 9CI*
$C_{10}H_9BrN_2O$ M 253.0 Alkaloid from the marine sponge *P. hyalinus*. Mp 148-150°.

Nitrile: [152213-61-1]. *6-Bromo-1H-indole-3-acetonitrile, 9CI. 6-Bromo-3-(cyanomethyl) indole*
$C_{10}H_7BrN_2$ M 235.0 Alkaloid from the marine sponge *P. hyalinus*. Mp 114-115°.

Rasmussen, T. *et al*, *J. Nat. Prod.*, 1993, **56**, 1553.

1-Bromo-3-iodobicyclo[1.1.1]pentane B-1-00305

[136863-39-3]

C_5H_6BrI M 272.9
Cryst. by subl. Mp 125-127°.

Della, E.W. *et al*, *J.O.C.*, 1994, **59**, 2986 (*synth, pmr, cmr, ms*)

3′-Bromo-2-iodobiphenyl B-1-00306

$C_{12}H_8BrI$ M 359.0
Oil. $Bp_{0.3}$ 145-147°.

Gioanola, M. *et al*, *Tetrahedron*, 1995, **51**, 2039 (*synth, pmr, ms*)

2-Bromo-3-iodothiophene B-1-00307

[24287-92-1]

C_4H_2BrIS M 288.9
Liq. Bp_{10} 106-109°.

Gronowitz, S. *et al*, *Acta Chem. Scand.*, 1969, **23**, 2207 (*synth, pmr*)

2-Bromo-4-iodothiophene B-1-00308

[60729-35-3]

C_4H_2BrIS M 288.9
Liq. Bp_{10} 106-108°.

Gronowitz, S. *et al*, *Acta Chem. Scand., Ser. B*, 1976, **30**, 505 (*synth, pmr*)
Wellmar, U. *et al*, *J. Het. Chem.*, 1995, **32**, 1159 (*synth*)

2-Bromo-5-iodothiophene B-1-00309

[29504-81-2]

C_4H_2BrIS M 288.9
Liq. Bp_{17} 116-118°.

Suzuki, H. *et al*, *Bull. Inst. Chem. Res., Kyoto Univ.*, 1974, **52**, 561 (*synth*)
Gronowitz, S. *et al*, *Acta Chem. Scand., Ser. B*, 1976, **30**, 423 (*synth, pmr*)

3-Bromo-2-iodothiophene B-1-00310

[60404-24-2]

C_4H_2BrIS M 288.9
Liq. Bp_9 108-110°.

Gronowitz, S. *et al*, *Acta Chem. Scand., Ser. B*, 1976, **30**, 423 (*synth, pmr*)
Meunier, P. *et al*, *Can. J. Chem.*, 1977, **55**, 3901 (*synth, pmr*)

3-Bromo-4-iodothiophene B-1-00311

[73882-41-4]

C_4H_2BrIS M 288.9
Liq. $Bp_{3.5}$ 107-110°.

Gronowitz, S. *et al*, *J. Het. Chem.*, 1980, **17**, 171 (*synth, pmr, ms*)
Spagnolo, P. *et al*, *J.O.C.*, 1982, **47**, 3177 (*synth, pmr*)

4-Bromo-2-iodothiophene B-1-00312

[73882-40-3]

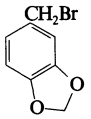
C_4H_2BrIS M 288.9
Liq. Bp_1 70-80°.

Gronowitz, S. *et al*, *Ark. Kemi*, 1960, **16**, 309 (*synth*)
Gronowitz, S. *et al*, *J. Het. Chem.*, 1980, **17**, 171 (*synth, pmr, ms*)

5-(Bromomethyl)-1,3-benzodioxole, 9CI B-1-00313

3,4-Methylenedioxybenzyl bromide

[2606-51-1]

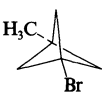


$C_8H_7BrO_2$ M 215.0
Cryst. (hexane). Mp 49-50° (45.5-47°).

Weinstein, B. *et al*, *J.O.C.*, 1976, **41**, 875 (*synth*)
van Oeveren, A. *et al*, *J.O.C.*, 1994, **59**, 5999 (*synth, pmr, cmr*)

1-Bromo-3-methylbicyclo[1.1.1]pentane B-1-00314

[137741-15-2]



C_6H_9Br M 161.0
Liq. Bp_{50} 80° (Kugelrohr).

Della, E.W. *et al*, *J.O.C.*, 1994, **59**, 2986 (*synth, prm, cmr, ms*)

3-Bromo-2-methyl-1,1′-biphenyl, 9CI B-1-00315

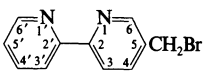
2-Bromo-6-phenyltoluene

$C_{13}H_{11}Br$ M 247.1
Oil.

Cullen, K.E. *et al*, *J.C.S. Perkin 1*, 1995, 2565 (*synth, pmr, ms*)

5-(Bromomethyl)-2,2′-bipyridine, 9CI B-1-00316

[98007-15-9]



$C_{11}H_9BrN_2$ M 249.1
Pale yellow solid or cryst. (hexane). Mp 72-73°.

Uenishi, J. *et al*, *J.O.C.*, 1993, **54**, 4382 (*synth, pmr, cmr, ms*)
Imperiali, B. *et al*, *J.O.C.*, 1993, **58**, 1613 (*synth, pmr, cmr, ir, uv*)

6-(Bromomethyl)-2,2′-bipyridine, 9CI B-1-00317

[83478-63-1]

$C_{11}H_9BrN_2$ M 249.1

Cryst. (hexane/C_6H_6). Mp 68-69° (65.5-67°).

Newkome, G.R. *et al*, *Inorg. Chem.*, 1983, **22**, 171 (*synth, pmr, ir, ms*)

Uenishi, J. *et al*, *J.O.C.*, 1993, **58**, 4382 (*synth, pmr*)

2-(Bromomethyl)-1-butanol, 9CI B-1-00318

3-Bromo-2-ethyl-1-propanol

$H_3CCH_2CH(CH_2OH)CH_2Br$

$C_5H_{11}BrO$ M 167.0

(±)-***form*** [155529-25-2]

Pale yellow oil.

Ihara, M. *et al*, *J.O.C.*, 1994, **59**, 5317 (*synth, ir, pmr*)

3-Bromo-3-methyl-2-butanone, 9CI B-1-00319

[2648-71-7]

$(H_3C)_2CBrCOCH_3$

C_5H_9BrO M 165.0

Liq. Bp_{150} 83-84°, Bp_{35} 50-54° (92% pure).

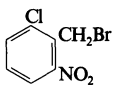
Favorsky, A., *J. Prakt. Chem.*, 1913, **88**, 641 (*synth*)

Takayanagi, H. *et al*, *J.C.S. Perkin 1*, 1995, 751 (*synth*)

2-(Bromomethyl)-1-chloro-3-nitrobenzene B-1-00320

2-Chloro-6-nitrobenzyl bromide

[56433-01-3]



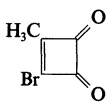
$C_7H_5BrClNO_2$ M 250.4

Mp 48-50°. Bp_{15} 134°.

Gindraux, L., *Helv. Chim. Acta*, 1929, **12**, 931.

3-Bromo-4-methyl-3-cyclobutene-1,2-dione B-1-00321

[130837-46-6]



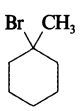
$C_5H_3BrO_2$ M 174.9

Yellow oil. $Bp_{0.5}$ 78-81°.

Liebesind, L.S. *et al*, *J.A.C.S.*, 1993, **115**, 9048 (*synth, ir, pmr*)

1-Bromo-1-methylcyclohexane, 9CI B-1-00322

[931-77-1]



$C_7H_{13}Br$ M 177.0

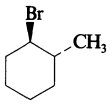
Liq. Bp 159-160°.

Landini, D. *et al*, *J.O.C.*, 1980, **45**, 3527 (*synth*)

Kim, S. *et al*, *J.O.C.*, 1988, **53**, 3111 (*synth*)

1-Bromo-2-methylcyclohexane, 9CI B-1-00323

[6294-39-9]



(1*RS*,2*RS*)-*form*

$C_7H_{13}Br$ M 177.0

(***1RS,2RS*)-*form*** [28046-85-7]

(±)-trans-*form*

Liq. Bp_{25} 73-74° (87% *trans*).

(***1RS,2SR*)-*form*** [28046-84-6]

(±)-cis-*form*

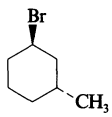
Liq. Bp_{40} 87° (>95% *cis*).

Schneider, H.-J. *et al*, *J.O.C.*, 1978, **43**, 3866 (*cmr*)

Kitching, W. *et al*, *J.O.C.*, 1982, **47**, 1893 (*synth, pmr*)

1-Bromo-3-methylcyclohexane, 9CI B-1-00324

[13905-48-1]



(1*RS*,3*RS*)-*form*

$C_7H_{13}Br$ M 177.0

(***1RS,3RS*)-*form*** [28046-89-1]

(±)-trans-*form*

Liq. Bp_{40} 84-86° (90% *trans*).

(***1RS,3SR*)-*form*** [28046-88-0]

(±)-cis-*form*

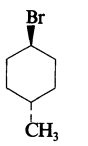
Liq. Bp_{20} 67-69° (85% *cis*).

Schneider, H.J. *et al*, *J.O.C.*, 1978, **43**, 3866 (*cmr*)

Kitching, W. *et al*, *J.O.C.*, 1982, **47**, 1893 (*synth, pmr*)

1-Bromo-4-methylcyclohexane, 9CI B-1-00325

[6294-40-2]



(1*RS*,4*RS*)-*form*

$C_7H_{13}Br$ M 177.0

(***1RS,4RS*)-*form*** [28046-91-5]

trans-*form*

Liq. Bp_{20} 69° (>95% *trans*).

(***1RS,4SR*)-*form*** [28046-90-4]

cis-*form*

Liq. Bp_{20} 72° (>95% *cis*).

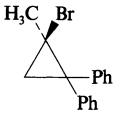
Kitching, W. *et al*, *J.O.C.*, 1982, **47**, 1893 (*synth, pmr*)

Olszowy, H.A. *et al*, *Organometallics*, 1984, **3**, 1676 (*synth, cmr*)

1-Bromo-1-methyl-2,2-diphenylcyclopropane, 8CI B-1-00326

1,1′-(2-Bromo-2-methylcyclopropylidene) bisbenzene, 9CI

[27468-37-7]



(*R*)-*form*

$C_{16}H_{15}Br$ M 287.1

(***R*)-*form*** [4542-82-9]

Cryst. Mp 82-83°. $[\alpha]_D^{25.5}$ −111.6 (c, 1.0 in $CHCl_3$).

(***S*)-*form*** [6526-76-7]

Cryst. Mp 84-85° (81-82°). $[\alpha]_D^{25.5}$ +111.6 (c, 1.0 in $CHCl_3$).

(±)-***form*** [10439-29-9]

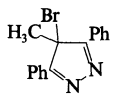
Pale yellow solid (MeOH). Mp 82-84°.

Walborsky, H.M. *et al*, *J.A.C.S.*, 1959, **81**, 5835; 1961, **83**, 2517; 1964, **86**, 3283 (*synth*)

Walborsky, H.M. *et al*, *J. Organomet. Chem.*, 1973, **51**, 31, 55 (*synth*)

4-Bromo-4-methyl-3,5-diphenyl-4*H*-pyrazole, 9CI B-1-00327

[159501-71-0]



$C_{16}H_{13}BrN_2$ M 313.1

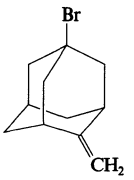
Yellow powder (CH_2Cl_2/pentane). Mp 130-132°.

Adam, W. *et al*, *J.O.C.*, 1994, **59**, 7067 (*synth, ir, pmr, uv, cmr*)

1-Bromo-4-methyleneadamantane B-1-00328

1-Bromo-4-methylenetricyclo[3.3.1.1^{3,7}]decane, 9CI

[155396-27-3]



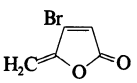
$C_{11}H_{15}Br$ M 227.1

Oil. n_D^{25} 1.5500.

Adcock, W. *et al*, *J.O.C.*, 1994, **59**, 1867 (*synth, pmr, cmr*)

4-Bromo-5-methylene-2(5*H*)-furanone B-1-00329

[132334-61-3]



$C_5H_3BrO_2$ M 174.9

Cryst. (hexane/Et_2O). Mp 59-61° dec.

de March, P. *et al*, *J.O.C.*, 1995, **60**, 1814 (*synth, ir, pmr, cmr, ms*)

2-Bromo-3-methylfuran B-1-00330

[64230-60-0]

C_5H_5BrO M 160.9
Bp_{60} 56-57°, Bp_{12} 28-30°.

▶ Polymerises explosively on exposure to air at 20°.

Prugh, J.D. *et al*, *J.O.C.*, 1964, **29**, 1991 (*synth, pmr, glc, haz*)
Takeda, A. *et al*, *Bull. Chem. Soc. Jpn.*, 1977, **50**, 1903 (*synth, ir, pmr*)
Bock, I. *et al*, *Tetrahedron*, 1990, **46**, 1199 (*synth, pmr*)

2-Bromo-4-methylfuran B-1-00331

[78259-59-3]

C_5H_5BrO M 160.9
Liq. Bp 138-144°.

Knight, D.W. *et al*, *J.C.S. Perkin 1*, 1981, 679 (*synth, ir, pmr*)

3-Bromo-2-methylfuran B-1-00332

[83457-06-1]

C_5H_5BrO M 160.9
Liq. Bp 124-127°.

Koyanagi, J. *et al*, *J. Het. Chem.*, 1994, **31**, 1093 (*synth, pmr, ms*)

4-Bromo-2-methylfuran B-1-00333

[24666-43-1]

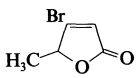
C_5H_5BrO M 160.9
Liq. Bp 132-134° (126-129°), Bp_{60} 60-62°.

Koyanagi, J. *et al*, *J. Het. Chem.*, 1994, **31**, 1093 (*synth, pmr, ms*)

4-Bromo-5-methyl-2(5*H*)-furanone, 9CI B-1-00334

3-Bromo-2-pentenolide

[130077-93-9]



$C_5H_5BrO_2$ M 176.9

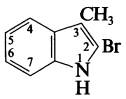
(±)-***form***
Cryst. (pentane). Mp 52-53°.

Shaw, E., *J.A.C.S.*, 1946, **68**, 2510 (*synth*)
Font, J. *et al*, *Tetrahedron*, 1990, **46**, 4407 (*synth*)
de March, P. *et al*, *J.O.C.*, 1995, **60**, 1814 (*synth*)

2-Bromo-3-methyl-1*H*-indole, 9CI B-1-00335

2-Bromoskatole

[1484-28-2]



C_9H_8BrN M 210.0
Cryst. (AcOH aq.). Mp 88-90°.

Hino, T. *et al*, *Chem. Pharm. Bull.*, 1967, **15**, 1800 (*synth, ir, uv*)
Mistry, A.G. *et al*, *Tet. Lett.*, 1986, **27**, 1051 (*synth*)

3-Bromo-2-methyl-1*H*-indole, 9CI B-1-00336

[1496-78-2]

C_9H_8BrN M 210.0
Cryst. (C_6H_6/hexane). Mp 90-91°.

Hinman, R.L. *et al*, *J.O.C.*, 1964, **29**, 1206 (*synth*)
Bucchi, V. *et al*, *Synthesis*, 1982, 1096 (*synth, pmr, ms*)

4-Bromo-2-methyl-1*H*-indole B-1-00337

C_9H_8BrN M 210.0
Pale yellow oil. $Bp_{0.01}$ 102°.

Picrate: Cryst. (EtOH). Mp 167.5-168°.

Piper, J.R. *et al*, *J. Het. Chem.*, 1966, **3**, 95 (*synth*)

5-Bromo-2-methyl-1*H*-indole, 9CI B-1-00338

[1075-34-9]

C_9H_8BrN M 210.0
Mp 93-96°. Bp_2 132-133.5°.

Colo, V. *et al*, *Farmaco, Ed. Sci.*, 1954, **9**, 611; *CA*, **49**, 14733c (*synth*)
Terent'ev, A.P. *et al*, *Zh. Obshch. Khim.*, 1959, **29**, 2541; *CA*, **54**, 10991i (*synth*)

5-Bromo-3-methyl-1*H*-indole, 9CI B-1-00339

5-Bromoskatole

[10075-48-6]

C_9H_8BrN M 210.0
Cryst. (2-propanol). Mp 79°.

Noland, W.E. *et al*, *J.O.C.*, 1967, **32**, 828 (*synth, ir, uv*)
Nagarathnam, D. *et al*, *Synth. Commun.*, 1993, **23**, 2011 (*synth*)

5-Bromo-7-methyl-1*H*-indole B-1-00340

[15936-81-9]

C_9H_8BrN M 210.0
Bp_{10} 120-125°.

Picrate: [15936-82-0].
Orange needles. Mp 155°.

Ambekar, S.Y. *et al*, *Monatsh. Chem.*, 1967, **98**, 798 (*synth*)

6-Bromo-2-methyl-1*H*-indole, 9CI B-1-00341

[6127-19-1]

C_9H_8BrN M 210.0
Cryst. (C_6H_6/petrol). Mp 113-114°.

Piper, J.R. *et al*, *J. Het. Chem.*, 1966, **3**, 95 (*synth*)
Ohta, T. *et al*, *Heterocycles*, 1987, **26**, 2817 (*synth*)

7-Bromo-5-methyl-1*H*-indole B-1-00342

[15936-79-5]

C_9H_8BrN M 210.0
Bp_{10} 165°.

Picrate: [15936-80-8].
Blue-red needles. Mp 149-150°.

Ambekar, S.Y. *et al*, *Monatsh. Chem.*, 1967, **98**, 798 (*synth*)

5-Bromo-2-methyl-2-pentene, 9CI B-1-00343

[2270-59-9]

$(H_3C)_2C{=}CHCH_2CH_2Br$

$C_6H_{11}Br$ M 163.0
Intermed. for synthesis of bisabolenes. Liq. Bp 155-156°, Bp_{75} 80-81°. n_D^{20} 1.4758. Darkens on exp. to light.

Ruzicka, L. *et al*, *Helv. Chim. Acta*, 1932, **15**, 3 (*synth*)
Willimann, L. *et al*, *Helv. Chim. Acta*, 1952, **35**, 2401 (*synth*)
Sarycheva, I.K. *et al*, *Zh. Obshch. Khim.*, 1955, **25**, 2001; *J. Gen. Chem. USSR (Engl. Transl.)*, 1955, **25**, 1949 (*synth*)
Julia, M. *et al*, *Bull. Soc. Chim. Fr.*, 1960, 1072 (*synth*)
Buchbauer, G., *Monatsh. Chem.*, 1978, **109**, 289 (*synth*)
Hudlicky, T. *et al*, *J.O.C.*, 1983, **48**, 5321 (*synth, pmr*)
Barua, N.C. *et al*, *Tetrahedron*, 1993, **49**, 2253 (*synth*)
Carpita, A. *et al*, *Synth. Commun.*, 1994, **24**, 3167 (*synth, pmr*)

(Bromomethyl)phosphonous diamide, 9CI B-1-00344

$BrCH_2P(NH_2)_2$

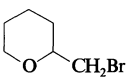
CH_6BrN_2P M 156.9

N,N,N′,N′-*Tetraisopropyl:* [124862-13-1]. P-(*Bromomethyl*)-N,N,N′,N′-*tetraisopropylphosphonous diamide.* (*Bromomethyl*)*phosphonous bis*(*diisopropylamide*)
$C_{13}H_{30}BrN_2P$ M 325.2 Needles. Mp 56-58°.

Kolodyazhnyi, O.I. *et al*, *Zh. Obshch. Khim.*, 1990, **60**, 1722; *J. Gen. Chem. USSR (Engl. Transl.)*, 1990, **60**, 1536 (*synth, pmr, cmr, P-31 nmr*)

2-(Bromomethyl)tetrahydro-2*H*-pyran B-1-00345

[34723-82-5]



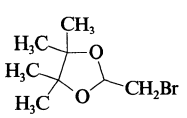
$C_6H_{11}BrO$ M 179.0
n_D^{20} 1.4890.

(±)-***form***
Liq. Bp_{17} 75-79°.

[130232-48-3, 130233-15-7, 130233-16-8]

Mas, J.-M. *et al*, *Synth. Commun.*, 1992, **22**, 2187 (*synth*)

2-(Bromomethyl)-4,4,5,5-tetramethyl-1,3-dioxolane B-1-00346



$C_8H_{15}BrO_2$ M 223.1

Oil.

Conole, G. *et al*, *J.C.S. Perkin 1*, 1995, 1825 (*synth, pmr, ms, cmr*)

1-(Bromomethyl)-2-(trifluoromethyl)benzene, 9CI B-1-00347

2-(Trifluoromethyl)benzyl bromide. α¹-Bromo-α,α,α-trifluoro-o-xylene. 2-(Bromomethyl) benzotrifluoride

[395-44-8]

$C_8H_6BrF_3$ M 239.0
d 1.57. $Bp_{7.5}$ 72°.

Filler, R. *et al*, *J.O.C.*, 1960, **25**, 733 (*synth*)

1-(Bromomethyl)-3-(trifluoromethyl)benzene B-1-00348

3-(Trifluoromethyl)benzyl bromide. α¹-Bromo-α,α,α-trifluoro-m-xylene. 3-(Bromomethyl) benzotrifluoride

[402-23-3]

$C_8H_6BrF_3$ M 239.0
d 1.56. Bp_4 69°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 916D.

Filler, R. *et al*, *J.O.C.*, 1960, **25**, 733 (*synth*)

1-(Bromomethyl)-4-(trifluoromethyl)benzene B-1-00349

α¹-Bromo-α,α,α-trifluoro-p-xylene. 4-(Trifluoromethyl)benzyl bromide. 4-(Bromomethyl)benzotrifluoride

[402-49-3]

$C_8H_6BrF_3$ M 239.0
d 1.55. Mp 31-34°. Bp_5 65-66°.

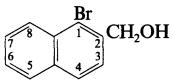
Aldrich Library of FT-IR Spectra, 1st edn., **3**, 919C.

Hass, H.B. *et al*, *J.A.C.S.*, 1949, **71**, 1767 (*synth*)

1-Bromo-2-naphthalenemethanol, 9CI B-1-00350

1-Bromo-2-(hydroxymethyl)naphthalene

[76635-70-6]



$C_{11}H_9BrO$ M 237.0
Cryst. (EtOH). Mp 103-104°.

Hebbelynck, M.G. *et al*, *Bull. Soc. Chim. Belg.*, 1952, **61**, 635 (*synth*)

Smith, J.G. *et al*, *J.O.C.*, 1986, **51**, 3762 (*synth, ir, pmr*)

Grissom, J.W. *et al*, *J.O.C.*, 1994, **59**, 7876 (*synth, ir, pmr, cmr*)

3-Bromo-2-naphthalenemethanol B-1-00351

3-Bromo-2-(hydroxymethyl)naphthalene

[38399-19-8]

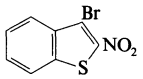
$C_{11}H_9BrO$ M 237.0
Cryst. (toluene/hexane). Mp 113-115° (95-100°).

Staab, H.A. *et al*, *Chem. Ber.*, 1972, **105**, 2290 (*synth*)

Smith, J.G. *et al*, *J.O.C.*, 1986, **51**, 3762 (*synth, ir, pmr*)

3-Bromo-2-nitrobenzo[*b*]thiophene B-1-00352

[17402-78-7]



$C_8H_4BrNO_2S$ M 258.0
Cryst. (EtOH). Mp 162.0-162.8°.

Van Zyl, G. *et al*, *Can. J. Chem.*, 1966, **44**, 2283 (*synth*)

Boswell, D.E. *et al*, *J. Het. Chem.*, 1968, **5**, 69 (***synth***)

3-Bromo-5-nitro-2-naphthylamine B-1-00353

6-Amino-7-bromo-1-nitronaphthalene

$C_{10}H_7BrN_2O_2$ M 267.0
Red solid.

Kelly, T.R. *et al*, *J.A.C.S.*, 1994, **116**, 7072 (*synth, pmr*)

3-Bromo-8-nitro-2-naphthylamine B-1-00354

7-Amino-6-bromo-1-nitronaphthalene

$C_{10}H_7BrN_2O_2$ M 267.0
Red powder (Et_2O/petrol). Mp 180-182°.

Kelly, T.R. *et al*, *J.A.C.S.*, 1994, **116**, 7072 (*synth, pmr*)

2-Bromo-2-nitro-1-propanol B-1-00355

Debropol, BAN, INN. *BTS 7706*

[24403-04-1]

$H_3CCBr(NO_2)CH_2OH$

$C_3H_6BrNO_3$ M 183.9
Shows bactericidal props. Antiseptic, preservative.

(±)-***form***
Needles. Mp 42°.

Ac: [53607-62-8].
$C_5H_8BrNO_4$ M 226.0 $Bp_{1.4}$ 75°.

Henry, *Chem. Zentralbl.*, 1897, **II**, 338 (*synth*)

Clark, N.G. *et al*, *J. Med. Chem.*, 1974, **17**, 977 (*acetate*)

6-Bromo-1,1,1,2,2,3,3,4,4-nonafluorohexane B-1-00356

[38436-14-5]

$F_3C(CF_2)_3CH_2CH_2Br$

$C_6H_4BrF_9$ M 326.9
Bp 93-94°, Bp_{35} 42°. n_D^{25} 1.3330.

Kim, Y.K. *et al*, *J.O.C.*, 1973, **38**, 1615.

9-Bromononanal, 9CI B-1-00357

[124388-97-2]

$BrCH_2(CH_2)_7CHO$

$C_9H_{17}BrO$ M 221.1
Solid or oil. Mp 27°. $Bp_{0.5}$ 105-110°.

Bhalerao, U.T. *et al*, *Indian J. Chem., Sect. B*, 1989, **28**, 579 (*synth, ir, pmr*)

U.K. Pat., 2 237 018, (1991); *CA*, **115**, 248092 (*synth*)

Bestmann, H.J. *et al*, *Synthesis*, 1994, 1257 (*synth, pmr*)

9-Bromo-1-nonanol, 9CI B-1-00358

[55362-80-6]

$BrCH_2(CH_2)_7CH_2OH$

$C_9H_{19}BrO$ M 223.1
Plates (petrol); needles (hexane). Mp 33.5°. Bp_2 125-126°.

Ac: [53596-82-0].
$C_{11}H_{21}BrO_2$ M 265.1 $Bp_{0.5}$ 122-123°.

Chuit, P. *et al*, *Helv. Chim. Acta*, 1929, **12**, 463 (*synth*)

Butenandt, A. *et al*, *Annalen*, 1962, **658**, 39 (*synth*)

Hendry, L.B. *et al*, *J. Chem. Ecol.*, 1975, **1**, 317 (*synth, pmr*)

Camps, F. *et al*, *Org. Prep. Proced. Int.*, 1983, **15**, 63 (*synth, ir, pmr, cmr*)

Weiler, L. *et al*, *Can. J. Chem.*, 1992, **70**, 1436; 1994, **72**, 150 (*synth, ir, pmr, ms*)

Bestmann, H.J. *et al*, *Synthesis*, 1994, 1257 (*synth*)

9-Bromo-1-nonene, 9CI B-1-00359

[89359-54-6]

$H_2C{=}CH(CH_2)_6CH_2Br$

$C_9H_{17}Br$ M 205.1
Liq. Bp_{45} 131-132°, Bp_{15} 110-115°.

Gaubert, P. *et al*, *J.C.S.*, 1937, 1971 (*synth*)

Johnson, D.K. *et al*, *Synth. Commun.*, 1994, **24**, 1557 (*synth, pmr, cmr*)

8-Bromooctanal, 9CI B-1-00360

[92540-33-5]

$BrCH_2(CH_2)_6CHO$

$C_8H_{15}BrO$ M 207.1
Liq. $Bp_{0.5}$ 82-86°.

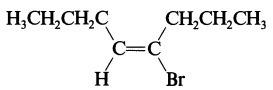
Di-Me acetal: [92540-34-6]. *8-Bromo-1,1-dimethoxyoctane, 9CI*
$C_{10}H_{21}BrO_2$ M 253.1 Oil. $Bp_{0.05}$ 84°.

Wiley, R.A. *et al*, *J. Med. Chem.*, 1989, **32**, 1319 (*acetal*)

Tolstikov, A.G. *et al*, *Khim. Prir. Soedin.*, 1991, 707; *Chem. Nat. Compd. (Engl. Transl.)*, 1991, 624 (*synth, pmr*)

Bestmann, H.J. *et al*, *Synthesis*, 1994, 1257 (*synth, pmr*)

4-Bromo-4-octene B-1-00361



(*E*)-*form*

$C_8H_{15}Br$ M 191.1

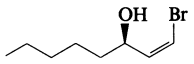
(***E*)-form** [24291-80-3]
cis-*form*
Liq.

(***Z*)-form** [24291-81-4]
trans-*form*
Liq.

Hudrlik, P.F. *et al*, *Tetrahedron*, 1983, **39**, 877 (*synth, ir, pmr*)

Kropp, P.J. *et al*, *J.O.C.*, 1994, **59**, 3102 (*synth, pmr*)

1-Bromo-1-octen-3-ol, 9CI B-1-00362



(*R*)-(*Z*)-*form*

$C_8H_{15}BrO$ M 207.1

(*R*)-(*Z*)-*form* [113428-14-1]
$[\alpha]_D^{25}$ +40.8 (c, 1.79 in $CHCl_3$).

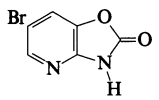
(*S*)-(*E*)-*form* [72243-93-7]
Oil. $[\alpha]_D^{24}$ +13.1 (c, 1.4 in MeOH) (100% op).

[120293-90-5]

Chen, S.-M.L. *et al*, *J.O.C.*, 1978, **43**, 3450 (*synth, ir, pmr*)
Noyori, R. *et al*, *J.A.C.S.*, 1984, **106**, 6717 (*synth, ir, pmr*)
Okamoto, S. *et al*, *Tet. Lett.*, 1987, **28**, 2033 (*synth*)
Matsumoto, T. *et al*, *Tet. Lett.*, 1988, **29**, 5685.

6-Bromooxazolo[4,5-*b*]pyridin-2(3*H*)-one, 9CI B-1-00363

[21594-52-5]



$C_6H_3BrN_2O_2$ M 215.0
Cryst. solid. Mp 234°.

Rüfenacht, K. *et al*, *Helv. Chim. Acta*, 1976, **59**, 1593 (*synth*)
Flouzat, C. *et al*, *J. Med. Chem.*, 1993, **36**, 497 (*synth, pmr*)

1-Bromo-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoroheptane B-1-00364

Perfluoroheptyl bromide

[375-88-2]

$F_3C(CF_2)_5CF_2Br$

C_7BrF_{15} M 448.9
Bp 123-124°. n_D^{25} 1.3010.

Haszeldine, R.N., *J.C.S.*, 1952, 4259.

Bromopentafluorobenzene, 9CI, 8CI B-1-00365

[344-04-7]

$(C_6F_5)Br$

C_6BrF_5 M 246.9
Liq. d^{20} 1.9503. Mp −31° (−29.9°). Bp 134-135°. n_D^{20} 1.4506. λ_{max} 243 nm (EtOH).

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 947D (*ir*)
Desirant, Y., *Bull. Soc. Chim. Belg.*, 1958, **67**, 676 (*synth, props*)
Nield, E. *et al*, *J.C.S.*, 1959, **166**, 169 (*synth, uv*)
Smithson, L.D. *et al*, *Org. Mass Spectrom.*, 1970, **4**, 1 (*ms*)
Rezvukhin, A.I. *et al*, *CA*, 1983, **98**, 16213f (*cmr*)
Bardin, V.V. *et al*, *J. Fluorine Chem.*, 1983, **23**, 67 (*synth, F-19 nmr*)

1-Bromo-2-pentanol, 9CI B-1-00366

[26818-03-1]

$H_3CCH_2CH_2CH(OH)CH_2Br$

$C_5H_{11}BrO$ M 167.0

(±)-*form*
Liq. Bp_{16-18} 77-79°.

Forgo, I. *et al*, *Pharm. Acta Helv.*, 1970, **45**, 227 (*synth*)
Kauffmann, T. *et al*, *Chem. Ber.*, 1982, **115**, 645 (*synth*)

2-Bromo-3-pentanol, 9CI B-1-00367

$H_3CCH_2CH(OH)CHBrCH_3$

$C_5H_{11}BrO$ M 167.0
Liq. Bp_{23} 74°. Mixt. of stereoisomers.

[63569-56-2, 63569-57-3]

House, H.O. *et al*, *J.A.C.S.*, 1955, **77**, 5083 (*synth, ir*)
Modro, A. *et al*, *J.O.C.*, 1977, **42**, 3673 (*synth, pmr, acetate*)

3-Bromo-2-pentanol B-1-00368

$H_3CCH_2CHBrCH(OH)CH_3$

$C_5H_{11}BrO$ M 167.0
Liq. Bp_{12} 58.5-60°. Mixt. of diastereoisomers.

House, H.O., *J.A.C.S.*, 1955, **77**, 5083 (*synth, ir*)

4-Bromo-1-pentanol, 9CI B-1-00369

[16103-56-3]

$H_3CCHBrCH_2CH_2CH_2OH$

$C_5H_{11}BrO$ M 167.0

(±)-*form*

Ac: [26923-92-2].
$C_7H_{13}BrO_2$ M 209.0 Liq. $Bp_{2.5}$ 65-68°.

Karger, M.H. *et al*, *J.O.C.*, 1971, **36**, 532 (*synth, pmr*)
Yadav, Y.K. *et al*, *J.O.C.*, 1986, **51**, 3373 (*synth, pmr*)

4-Bromo-2-pentanol, 9CI B-1-00370

[76137-48-9]

$H_3CCHBrCH_2CH(OH)CH_3$

$C_5H_{11}BrO$ M 167.0
Liq. Bp_{12} 78-79°. Mixt. of stereoisomers.

Ac: [76137-49-0].
$C_7H_{13}BrO_2$ M 209.0 Liq. $Bp_{4.5}$ 60-70°.

Brown, H.C. *et al*, *J.O.C.*, 1981, **46**, 930 (*synth*)

5-Bromo-1-pentanol, 9CI B-1-00371

[34626-51-2]

$BrCH_2(CH_2)_3CH_2OH$

$C_5H_{11}BrO$ M 167.0
Liq. $Bp_{0.5}$ 75-76°, $Bp_{0.2}$ 53-56°.

Ac: [15848-22-3].
$C_7H_{13}BrO_2$ M 209.0 Liq. Bp_{15} 110-115°, $Bp_{0.8}$ 60-67°.

Guindon, Y. *et al*, *J.O.C.*, 1987, **52**, 1680 (*synth*)
Lermer, L. *et al*, *Can. J. Chem.*, 1992, **70**, 1427 (*synth, ir, pmr, ms*)
Bestmann, H.J. *et al*, *Synthesis*, 1992, 1239 (*acetate*)
Manchand, P.S. *et al*, *Tetrahedron*, 1992, **48**, 9391 (*synth, ir, pmr, acetate*)

1-Bromo-2-pentanone, 9CI B-1-00372

Bromomethyl propyl ketone

[817-71-0]

$H_3CCH_2CH_2COCH_2Br$

C_5H_9BrO M 165.0
Oil. Bp_{50} 92-92.5°. n_D^{23} 1.4620.

Catch, J.R. *et al*, *J.C.S.*, 1948, 276 (*synth*)
Asinger, F. *et al*, *Annalen*, 1964, **672**, 156 (*synth*)
Eur. Pat., 427 480, (1991); *CA*, **115**, 135680 (*synth*)

3-Bromo-2-pentanone, 9CI B-1-00373

[815-48-5]

$H_3CCH_2CHBrCOCH_3$

C_5H_9BrO M 165.0

(±)-*form*
Oil. Bp_{50} 78-78.5°. n_D^{20} 1.4629.
▶ Lachrymator.

Borrows, E.T. *et al*, *J.C.S.*, 1946, 1083 (*synth*)
Asinger, F. *et al*, *Annalen*, 1964, **672**, 156 (*synth*)
Gassman, P.G. *et al*, *J.A.C.S.*, 1974, **96**, 5495 (*synth*)
Groesbeek, M. *et al*, *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1989, **108**, 427 (*synth, pmr*)
Boyd, R.E. *et al*, *Synth. Commun.*, 1995, **25**, 1045 (*synth, pmr*)

1-Bromo-3-phenylbicyclo[1.1.1]pentane, 9CI B-1-00374

[112043-92-2]

$C_{11}H_{11}Br$ M 223.1
Cryst. Mp 31-31.5°.

Della, E.W. *et al*, *J.O.C.*, 1988, **53**, 592; 1994, **59**, 2986 (*synth, pmr, cmr, ms*)

3-Bromo-4-phenyl-3-cyclobutene-1,2-dione, 9CI B-1-00375

[22315-46-4]

$C_{10}H_5BrO_2$ M 237.0
Pale yellow solid (CCl_4). Mp 128-129°.

Smutny, E.J. *et al*, *J.A.C.S.*, 1960, **82**, 1793 (*synth*)
Liebeskind, L.S. *et al*, *J.A.C.S.*, 1993, **115**, 9048 (*synth, ir, pmr*)

1-Bromo-7-phenylheptane B-1-00376

(*7-Bromoheptyl*)*benzene, 9CI*

[78573-85-0]

$Ph(CH_2)_6CH_2Br$

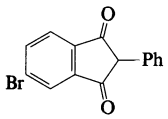
$C_{13}H_{19}Br$ M 255.1
Liq. $Bp_{1.5}$ 123-124°, $Bp_{0.05}$ 110-114°.

Collins, R.F. *et al*, *J.C.S.*, 1961, 1863 (*synth*)
Forth, M.A. *et al*, *J.O.C.*, 1994, **59**, 2616 (*synth, ir, pmr, cmr*)

5-Bromo-2-phenyl-1,3-indanedione B-1-00377

5-Bromo-2-phenyl-1H-indene-1,3(2H)-dione, 9CI. Isobromindione, INN. G/18. Uridion

[1470-35-5]



$C_{15}H_9BrO_2$ M 301.1

Uricosuric agent.

▶ LD_{50} (rat, orl) 150 mg/kg. Exp. reprod. effects (fetotoxic, other effects). NK5156000.

(±)-*form*

Violet-brown cryst. (MeOH). Mp 164-165°.

Dioxime:

$C_{15}H_{11}BrN_2O_2$ M 331.1 Mp 205-207° dec.

Perjessy, A. *et al, Tetrahedron*, 1971, **27**, 6159 (*ir*)

Fanelli, O. *et al, Arzneim.-Forsch.*, 1974, **24**, 1609; 1975, **25**, 873 (*tox, pharmacol*)

Islam, A.M. *et al, Bull. Chem. Soc. Jpn.*, 1974, **47**, 1274 (*synth*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 337.

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, UVJ400.

Lewis, R.J., *Reproductively Active Chemicals*, Van Nostrand Reinhold, 1991, UVJ400.

(2-Bromophenyl)phosphonous acid B-1-00378

2-(Dihydroxyphosphino)bromobenzene

$C_6H_6BrO_2P$ M 220.9

Dichloride: [5274-51-1].
$C_6H_4BrCl_2P$ M 257.8 Liq. Bp_1 80-82°.

Diamide: see P-(*2-Bromophenyl*)*phosphonous diamide, B-1-00379*

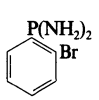
Chiswell, B. *et al, J.C.S.*, 1966, 417 (*dichloride*)

Talay, R. *et al, Z. Naturforsch., B*, 1981, **36**, 451 (*dichloride*)

Raskina, A.D. *et al, Zh. Obshch. Khim.*, 1985, **55**, 2262; *J. Gen. Chem. USSR (Engl. Transl.)*, 1985, **55**, 2008.

Werner, D. *et al, Z. Naturforsch., B*, 1987, **42**, 1110 (*dichloride, pmr, cmr, P-31 nmr*)

P-(2-Bromophenyl) phosphonous diamide, 9CI B-1-00379



$C_6H_8BrN_2P$ M 219.0

N,N,N′,N′-*Tetra-Me:* [82495-63-4]. P-(*2-Bromophenyl*)-N,N,N′,N′-*tetramethylphosphonous diamide.* (*2-Bromophenyl*)*phosphonous bis(dimethylamide)*
$C_{10}H_{16}BrN_2P$ M 275.1 Liq. $Bp_{0.06}$ 84-85°.

Drewelies, K. *et al, Angew. Chem., Int. Ed.*, 1982, **21**, 638; *Suppl.* 1416 (*synth, ir, pmr, cmr, P-31 nmr*)

Eritja, R. *et al, Tetrahedron*, 1990, **46**, 721 (*tetraethyl, P-31 nmr*)

P-(3-Bromophenyl) phosphonous diamide, 9CI B-1-00380

$C_6H_8BrN_2P$ M 219.0

N,N,N′,N′-*Tetra-Me:* [82495-64-5]. P-(*3-Bromophenyl*)-N,N,N′,N′-*tetramethylphosphonous diamide.* P-(*3-Bromophenyl*)*phosphonous bis(dimethylamide)*
$C_{10}H_{16}BrN_2P$ M 275.1 Liq. $Bp_{0.001}$ 75-77°.

Drewelies, K. *et al, Angew. Chem., Int. Ed.*, 1982, **21**, 638; *Suppl.* 1416 (*synth, ir, pmr, cmr, P-31 nmr*)

P-(4-Bromophenyl) phosphonous diamide, 9CI B-1-00381

$C_6H_8BrN_2P$ M 219.0

N,N,N′,N′-*Tetra-Me:* [95682-76-1]. P-(*4-Bromophenyl*)-N,N,N′,N′-*tetramethylphosphonous diamide.* (*4-Bromophenyl*)*phosphonous bis(dimethylamide)*
$C_{10}H_{16}BrN_2P$ M 275.1 Oil. $Bp_{0.04}$ 91-94°.

Woerz, H.J. *et al, Chem.-Ztg.*, 1984, **108**, 329 (*synth, pmr, P-31 nmr*)

1-Bromo-3-phenylpropane B-1-00382

(*3-Bromopropyl*)*benzene, 9CI, 8CI. 3-Phenylpropyl bromide*

[637-59-2]

$PhCH_2CH_2CH_2Br$

$C_9H_{11}Br$ M 199.0

Oil. Bp 219-220°, Bp_5 84-85°. n_D^{20} 1.55.

[51271-24-0, 60604-08-2, 66318-67-0, 74823-40-8, 117637-88-4]

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 892B.

Aldrich Library of NMR Spectra, 2nd edn., **1**, 776C.

Shimohigashi, Y. *et al, Bull. Chem. Soc. Jpn.*, 1976, **49**, 3280 (*synth*)

Hill, E.A. *et al, Org. Magn. Reson.*, 1981, **16**, 177 (*cmr*)

Kamijo, T. *et al, Chem. Pharm. Bull.*, 1983, **31**, 4189 (*synth*)

Hodge, P. *et al, J.C.S. Perkin 1*, 1984, 195 (*synth*)

Chattopadhyay, S. *et al, Indian J. Pure Appl. Phys.*, 1987, **25**, 456 (*ir, Raman, conformn*)

1-Bromo-2-(phenylthio)ethene B-1-00383

[(*2-Bromoethenyl*)*thio*]*benzene, 9CI.* (*2-Bromovinyl*)*phenyl sulfide*

[35088-66-5]

PhSCH=CHBr

C_8H_7BrS M 215.1

(*E*)-*form* [17101-82-5]
Liq. Bp_{16} 134.5-135.5°, Bp_4 100.5-101.5°.

S,S-*Dioxide:* [20408-25-7]. (*2-Bromovinyl*) *phenyl sulfone*
$C_8H_7BrO_2S$ M 247.1 Cryst. Mp 55-56°.

(*Z*)-*form* [17101-71-2]
Liq. $Bp_{0.04}$ 59-60°.

S,S-*Dioxide:* [52244-26-5].
Cryst. Mp 39-40°.

Angeletti, E. *et al, Gazz. Chim. Ital.*, 1957, **87**, 1086 (*synth*)

Shainyan, B.A. *et al, Zh. Org. Khim.*, 1989, **25**, 68; *J. Org. Chem. USSR (Engl. Transl.)*, 1989, **25**, 61 (*synth*)

Cardellicchio, C. *et al, Gazz. Chim. Ital.*, 1991, **121**, 11 (*synth*)

Bruncko, M. *et al, J.O.C.*, 1994, **59**, 7921 (*dioxide, synth, pmr, cmr*)

2-Bromo-1-phenyl-2-triphenylphosphoranylideneethanone, 9CI B-1-00384

[3201-60-3]

$Ph_3P{=}CBrCOPh$

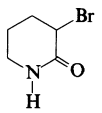
$C_{26}H_{20}BrOP$ M 459.3
Solid. Mp 151-152° dec.

Speziale, J. *et al, J.A.C.S.*, 1963, **85**, 2790 (*synth*)

Speziale, J. *et al, J.O.C.*, 1963, **28**, 465 (*synth*)

Braga, A.L. *et al, Synth. Commun.*, 1989, **19**, 2877 (*use*)

3-Bromo-2-piperidinone B-1-00385

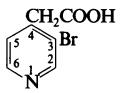


C_5H_8BrNO M 178.0

(±)-*form*
Cryst. ($CHCl_3$). Mp 147° (135-137°).

Uchikawa, O. *et al, J. Het. Chem.*, 1994, **31**, 1545 (*synth, pmr*)

3-Bromo-4-pyridineacetic acid B-1-00386



$C_7H_6BrNO_2$ M 216.0

Me ester: [162615-12-5].
$C_8H_8BrNO_2$ M 230.0 Pale yellow oil.

Et ester: [51054-99-0].
$C_9H_{10}BrNO_2$ M 244.0 Oil. $Bp_{0.06}$ 91-95°.

Nitrile: [142892-31-7]. *3-Bromo-4-*(*cyanomethyl*)*pyridine*
$C_7H_5BrN_2$ M 197.0 Mp 93-94°.

Hansen, J.F. *et al, J. Het. Chem.*, 1973, **10**, 711 (*Et ester*)

Bremner, D.H. *et al, Synthesis*, 1992, 528 (*nitrile*)

Bracher, F. *et al, Annalen*, 1995, 645 (*Me ester*)

5-Bromo-3-pyridineacetic acid, 9CI B-1-00387

[39891-12-8]

$C_7H_6BrNO_2$ M 216.0
Mp 184-185°.

Nitrile: [39891-08-2]. *3-Bromo-5-*(*cyanomethyl*)*pyridine*

$C_7H_5BrN_2$ M 197.0 Mp 76.5-77°.

Carlson, L.A. *et al*, *Acta Pharm. Suec.*, 1972, **9**, 411; *CA*, **78**, 58202u (*synth, nitrile*)

6-Bromo-3-pyridinecarboxaldehyde, 9CI B-1-00388

2-Bromo-5-formylpyridine

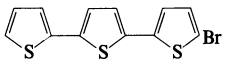
[149806-06-4]

C_6H_4BrNO M 186.0
Mp 100°.

Vögtle, F. *et al*, *Synthesis*, 1994, 87 (*synth, pmr, cmr, ms*)

5-Bromo-2,2′:5′,2″-terthiophene, 9CI B-1-00389

[94581-95-0]



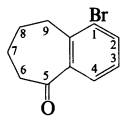
$C_{12}H_7BrS_3$ M 327.2
Yellow solid (hexane). Mp 141-142° (136-137.5°).

Morand, P. *et al*, *Tetrahedron*, 1988, **44**, 2403 (*synth, ms, cmr*)
Bäuerle, P. *et al*, *Synthesis*, 1993, 1099 (*synth, pmr*)

1-Bromo-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one, 9CI B-1-00390

6-Bromo-1-benzosuberone

[87779-79-1]



$C_{11}H_{11}BrO$ M 239.1
Oil. Bp_{12} 174°, $Bp_{0.12}$ 101-105°.

Gruber, R. *et al*, *Bull. Soc. Chim. Fr., Part II*, 1983, 96 (*synth, pmr, uv, ir*)
Combs, D.W. *et al*, *Synth. Commun.*, 1994, **24**, 2777 (*synth, pmr*)

3-Bromo-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one, 9CI B-1-00391

8-Bromo-1-benzosuberone

[87779-78-0]

$C_{11}H_{11}BrO$ M 239.1
Off-white powder. Mp 28-30°. Bp_{15} 184°.

2,4-Dinitrophenylhydrazone: [22647-90-1]. Orange needles. Mp 243°.

Gruber, R. *et al*, *Bull. Soc. Chim. Fr., Part II*, 1983, 96 (*synth, pmr, uv, ir*)
Combs, D.W. *et al*, *Synth. Commun.*, 1994, **24**, 2777 (*synth, pmr*)

6-Bromo-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one, 9CI B-1-00392

2-Bromo-1-benzosuberone

[19844-70-3]

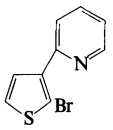
$C_{11}H_{11}BrO$ M 239.1

(±)-*form*
Bp_1 140-142°. n_D^{25} 1.5940.

Tarbell, D.S. *et al*, *J.A.C.S.*, 1952, **74**, 6263 (*synth*)
Khanna, J.M. *et al*, *Indian J. Chem.*, 1968, **6**, 6 (*synth*)

2-(2-Bromo-3-thienyl)pyridine B-1-00393

2-Bromo-3-(2-pyridinyl)thiophene



C_9H_6BrNS M 240.1

Zhang, Y. *et al*, *J. Het. Chem.*, 1995, **32**, 435 (*synth, pmr, cmr*)

2-(5-Bromo-3-thienyl)pyridine B-1-00394

2-Bromo-4-(2-pyridinyl)thiophene

C_9H_6BrNS M 240.1
Mp 36-37°.

Zhang, Y. *et al*, *J. Het. Chem.*, 1995, **32**, 435 (*synth, pmr, cmr*)

3-(2-Bromo-3-thienyl)pyridine B-1-00395

2-Bromo-3-(3-pyridinyl)thiophene

C_9H_6BrNS M 240.1

Zhang, Y. *et al*, *J. Het. Chem.*, 1995, **32**, 435 (*synth, pmr, cmr*)

3-(5-Bromo-3-thienyl)pyridine, 9CI B-1-00396

2-Bromo-4-(3-pyridinyl)thiophene

[166450-99-3]

C_9H_6BrNS M 240.1
Cryst. (hexane). Mp 52-54°.

Zhang, Y. *et al*, *J. Het. Chem.*, 1995, **32**, 435 (*synth, pmr, cmr*)

4-(2-Bromo-3-thienyl)pyridine B-1-00397

2-Bromo-3-(4-pyridinyl)thiophene

C_9H_6BrNS M 240.1
Mp 56.5-58.5°.

Zhang, Y. *et al*, *J. Het. Chem.*, 1995, **32**, 435 (*synth, pmr, cmr*)

4-(5-Bromo-3-thienyl)pyridine B-1-00398

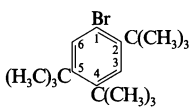
2-Bromo-4-(4-pyridinyl)thiophene

C_9H_6BrNS M 240.1
Cryst. (petrol). Mp 62-64°.

Gronowitz, S. *et al*, *Acta Chem. Scand.*, 1992, **46**, 654 (*synth*)
Zhang, Y. *et al*, *J. Het. Chem.*, 1995, **32**, 435 (*synth, pmr, cmr*)

1-Bromo-2,4,5-tri-*tert*-butylbenzene B-1-00399

1-Bromo-2,4,5-tris(1,1-dimethylethyl)benzene



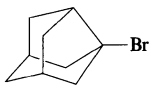
$C_{18}H_{29}Br$ M 325.3
Cryst. Mp 77°.

Dehmlow, E.V. *et al*, *Tetrahedron*, 1995, **51**, 3755 (*synth, pmr*)

3-Bromotricyclo[3.3.1.0^{3,7}]nonane B-1-00400

3a-Bromooctahydro-2,5-methanopentalene, 9CI. 3-Bromonoradamantane

[142761-44-2]



$C_9H_{13}Br$ M 201.1
Cryst. Mp 101.6°.

Olah, G.A. *et al*, *J.A.C.S.*, 1993, **115**, 10728 (*synth, ms, pmr, cmr*)

13-Bromo-1-tridecanol, 9CI B-1-00401

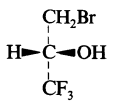
[116754-58-6]

$BrCH_2(CH_2)_{11}CH_2OH$

$C_{13}H_{27}BrO$ M 279.2
Mp 56-57°.

Mori, K. *et al*, *Annalen*, 1994, 695 (*synth, pmr*)

3-Bromo-1,1,1-trifluoro-2-propanol, 9CI B-1-00402



(*R*)-*form*

$C_3H_4BrF_3O$ M 192.9

(*R*)-*form* [160706-70-7]
Liq. Bp 122-123°. $[\alpha]_D^{22}$ −51.06 (neat) (96% ee).

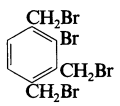
(±)-*form*
Liq. with slightly acrid odour. d_{20}^{20} 186. Mp −3.0°. $Bp_{743.3}$ 124.5°. n_D^{20} 1.4009.

α-Naphthylurethane: Cryst. solid. Mp 134.2-134.7°.

[88378-50-1]

McBee, E.T. *et al*, *J.A.C.S.*, 1952, **74**, 3022 (*synth*)
Ramachandran, P.V. *et al*, *J.O.C.*, 1995, **60**, 41 (*synth, ir, pmr, cmr, F-19 nmr*)

2-Bromo-1,3,4-tris(bromomethyl)benzene B-1-00403



$C_9H_8Br_4$ M 435.7
Cryst. (hexane). Mp 98-100°.

Tal, D.M. *et al*, *Tetrahedron*, 1995, **51**, 3823 (*synth, pmr*)

1-Bromoundecane, 9CI B-1-00404

Undecyl bromide

[693-67-4]

$H_3C(CH_2)_9CH_2Br$

$C_{11}H_{23}Br$ M 235.2
Liq. d 1.05. Mp −9°. Bp_{18} 137-138°. n_D^{20} 1.46.

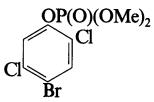
Lumb, P.B. *et al*, *J.C.S.*, 1952, 5032 (*synth*)
McLafferty, F.W. *et al*, *Anal. Chem.*, 1962, **34**, 2 (*ms*)

McKillop, A. *et al*, *J.O.C.*, 1969, **34**, 1172 (*synth*)
Cambie, R.C. *et al*, *J.C.S. Perkin 1*, 1981, 2608 (*synth*)

Bromoxon B-1-00405

4-Bromo-2,5-dichlorophenyl dimethyl phosphate, 9CI. Bromophos-oxon

[4855-62-3]



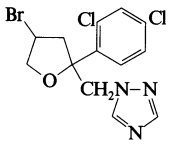
$C_8H_8BrCl_2O_4P$ M 349.9
Mp 64°.

Ger. Pat., 1 197 675, (1965); *CA*, **64**, 3421b (*synth*)

Bromuconazole, BSI B-1-00406

1-[[4-Bromo-2-(2,4-dichlorophenyl)tetrahydro-2-furanyl]methyl]-1H-1,2,4-triazole, 9CI. 1-[4-Bromo-2-(2,4-dichlorophenyl) tetrahydrofurfuryl]-1H-1,2,4-triazole. Bromoconazole. LS 860263

[116255-48-2]



$C_{13}H_{12}BrCl_2N_3O$ M 377.0
Sterol demethylation inhibitor. Antifungal agent. Cryst. Mp 84° (96°), Mp 104°. Mps given are for two (unspecified) diastereoisomers.

▶ LD_{50} (rat, orl) 365 mg/kg. XZ4130000.

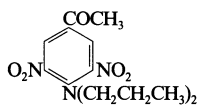
[114544-80-8, 114544-81-9, 135417-64-0]

Eur. Pat., 246 982, (1987) (*Rhône-Poulenc*); *CA*, **109**, 93016s (*synth, activity*)
Eur. Pat., 258 161, (1988) (*Rhône-Poulenc*); *CA*, **109**, 110440v (*synth, activity*)
Pepin, R. *et al*, *Br. Crop Prot. Conf. - Pests Dis., Proc.*, 1990, 439 (*activity, props*)
Pesticide Manual, 10th edn., 1994, No. 84.

Bulab B-1-00407

1-[4-(Dipropylamino)-3,5-dinitrophenyl] ethanone, 9CI. 4'-(Dipropylamino)-3',5'-dinitroacetophenone

[52129-71-2]



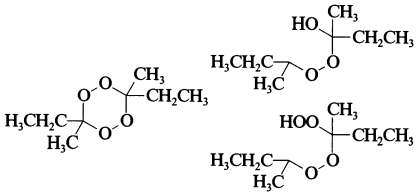
$C_{14}H_{19}N_3O_5$ M 309.3
Herbicide.

U.S. Pat., 3 933 472, (1976); *CA*, **84**, 106378d (*synth, use*)

2-Butanone peroxide, 9CI B-1-00408

Butanox. MEKP

[1338-23-4]



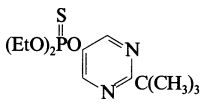
Said to be a mixture of 3 components but structural evidence is not convincing. Polymerisation initiator, cross linking agent for polyester adhesives. Commercial product is available as a 60% soln. in dimethyl phthalate with an available oxygen content of approx. 11%.

Manly, T.D. *et al*, *Ind. Chem.*, 1956, **32**, 271; *CA*, **50**, 15991a (*props, use*)
U.K. Pat., 827 511, (1960); *CA*, **54**, 12997d (*synth*)
U.S. Pat., 3 076 852, (1963); *CA*, **59**, 11257g (*synth*)
Rosso, J.C. *et al*, *C. R. Hebd. Seances Acad. Sci. Ser. C*, 1977, **284**, 199 (*hplc*)
Zhao, Z. *et al*, *CA*, 1990, **113**, 232671x (*synth, use*)

Butathiofos B-1-00409

O-[*2-(1,1-Dimethylethyl)-5-pyrimidinyl*] O,O-*diethylphosphorothioate, 9CI. Butathiophos*

[90338-20-8]



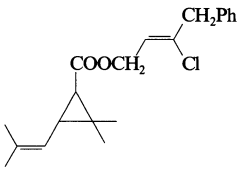
$C_{12}H_{21}N_2O_3PS$ M 304.3
Insecticide. Superseded.

U.S. Pat., 4 429 125, (1984); *CA*, **100**, 210153m (*synth, use*)
Ger. Pat., 3 538 912, (1985); *CA*, **107**, 59258w (*synth, use*)
Pesticide Manual, 9th edn., 1991, 1523.

Butethrin B-1-00410

3-Chloro-4-phenyl-2-butenyl 2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylate, 9CI

[28288-05-3]



$C_{20}H_{25}ClO_2$ M 332.8
Insecticide. $Bp_{0.12}$ 142-145°. Stereoisomeric mixt.

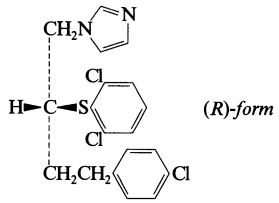
[32468-22-7, 33648-40-7, 33648-41-8]

Sota, K. *et al*, *Agric. Biol. Chem.*, 1971, **35**, 968 (*synth, use*)

Butoconazole, BAN, INN B-1-00411

1-[4-(4-Chlorophenyl)-2-[(2,6-dichlorophenyl) thio]butyl]-1H-imidazole, 9CI. Butaconazole

[67085-13-6]



(*R*)-*form*

$C_{19}H_{17}Cl_3N_2S$ M 411.7
Antifungal agent. Launched 1986.

(*R*)-*form*

Nitrate: [151909-77-2].
Cryst. (MeOH/EtOAc). Mp 123-125°. $[\alpha]_D^{25}$ −23.26 (c, 0.4 in EtOH).

(*S*)-*form*

Nitrate: [151909-75-0].
Cryst. (EtOAc/Et_2O). Mp 120-124°. $[\alpha]_D^{25}$ +22.68 (c, 0.4 in EtOH).

(±)-*form* [64872-76-0]
Cryst. (cyclohexane). Mp 68-70.5°.

Nitrate: [64872-77-1]. ***Butoconazole nitrate, USAN. Femstat. RS 35887-00-10-3***
Blades (Me_2CO/EtOAc). Mp 162-163°.

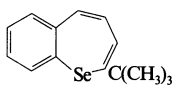
[67085-14-7, 82382-24-9]

Walker, K.A.M. *et al*, *J. Med. Chem.*, 1978, **211**, 840 (*synth, pmr*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, London, 1982/1989, 16554.
Odds, F.C. *et al*, *J. Antimicrob. Chemother.*, 1984, **14**, 105 (*props*)
Matthews, T., *J. Reprod. Med.*, 1986, **31**, 655 (*pharmacol*)
Rotstein, D.M. *et al*, *Tetrahedron: Asymmetry*, 1993, **4**, 1521 (*synth*)

2-*tert*-Butyl-1-benzoselenepin B-1-00412

2-(1,1-Dimethylethyl)-1-benzoselenepin, 9CI

[153140-94-4]



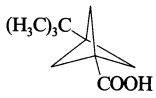
$C_{14}H_{16}Se$ M 263.2
Viscous orange-red oil. Other homologues also prepd. Me homologue could not be obt.

Sashida, H. *et al*, *Chem. Pharm. Bull.*, 1995, **43**, 19 (*synth, pmr*)

3-*tert*-Butylbicyclo[1.1.1] pentane-1-carboxylic acid B-1-00413

3-(1,1-Dimethylethyl)bicyclo[1.1.1]pentane-1-carboxylic acid, 9CI

[132663-73-1]



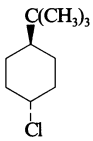
$C_{10}H_{16}O_2$ M 168.2
Cryst. by subl. Mp 155-157°.

Della, E.W. *et al*, *J.O.C.*, 1994, **59**, 2986 (*synth, ir, pmr, cmr, ms*)

1-*tert*-Butyl-4-chlorocyclohexane B-1-00414

1-Chloro-4-(1,1-dimethylethyl)cyclohexane

[62056-46-6]



(1*RS*,4*RS*)-*form*

$C_{10}H_{19}Cl$ M 174.7

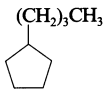
(***1RS,4RS*)-*form*** [13145-48-7]
trans-*form*
n_D^{20} 1.4656.

(***1RS,4SR*)-*form*** [13131-74-3]
cis-*form*
$Bp_{0.5}$ 38-40°. n_D^{20} 1.4694.

Eliel, E.L. *et al*, *J.A.C.S.*, 1968, **90**, 690 (*synth*)
Beckwith, A.L.J. *et al*, *Aust. J. Chem.*, 1983, **36**, 2123 (*synth*)
Roberts, B.P. *et al*, *J.C.S. Perkin 2*, 1994, 2411 (*synth, pmr*)

Butylcyclopentane B-1-00415

1-Cyclopentylbutane



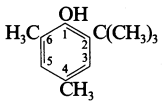
C_9H_{18} M 126.2
d^{20} 0.785. Fp −108.0°. Bp 156.6°. n_D^{20} 1.4316.

Adv. Chem. Ser., 1955, **15**, 382 (***props***)

2-*tert*-Butyl-4,6-dimethylphenol B-1-00416

2-(1,1-Dimethylethyl)-4,6-dimethylphenol, 9CI.
6-tert-Butyl-2,4-xylenol, 8CI

[1879-09-0]



$C_{12}H_{18}O$ M 178.2
Antioxidant, polymerisation inhibitor. Catalyst in phase transfer reactions. Fp 22.3°. Bp 249°, Bp_1 81.8°. n_D^{20} 1.5183.

Weinrich, W., *Ind. Eng. Chem.*, 1943, **35**, 264 (*synth, props*)
Pardee, W.A. *et al*, *Ind. Eng. Chem.*, 1944, **36**, 595 (*synth, props*)
Hedayatullah, M. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 2637 (*deriv*)
Eur. Pat., 281 992, (1988); *CA*, **110**, 118125n (*use*)
Jursic, B. *et al*, *Tetrahedron*, 1988, **44**, 6677 (*use*)

4-*tert*-Butyl-2,5-dimethylphenol B-1-00417

4-(1,1-Dimethylethyl)-2,5-dimethylphenol, 9CI.
4-tert-Butyl-2,5-xylenol, 8CI

[17696-37-6]

$C_{12}H_{18}O$ M 178.2
Used in the prepn. of musk and cosmetic compositions. $d_4^{26.7}$ 1.001. Fp 71.2°. Bp 264°, Bp_{20} 151°. n_D^{20} 1.5311.

Stevens, D.R. *et al*, *Ind. Eng. Chem.*, 1943, **35**, 655 (*synth*)
McKinley, J.B. *et al*, *Ind. Eng. Chem., Anal. Ed.*, 1944, **16**, 304 (*deriv synth*)
Pardee, W.A. *et al*, *Ind. Eng. Chem.*, 1944, **36**, 595 (*synth, prop*)
U.S. Pat., 4 880 775, (1989); *CA*, **112**, 185594u (*use*)

4-*tert*-Butyl-2,6-dimethylphenol B-1-00418

4-(1,1-Dimethylethyl)-2,6-dimethylphenol, 9CI.
4-tert-Butyl-2,6-xylenol, 8CI

[879-97-0]

$C_{12}H_{18}O$ M 178.2
Prisms. $d_4^{26.7}$ 0.959. Fp 84° (82.4°). Bp 248°, Bp_1 76.5°.

Tchitchibabine, A.E., *Bull. Soc. Chim. Fr.*, 1932, **51**, 1436 (*synth*)
Stevens, D.R., *Ind. Eng. Chem.*, 1943, **35**, 655 (*synth, prop*)
Pardee, W.A. *et al*, *Ind. Eng. Chem.*, 1944, **36**, 595 (*synth*)
Coggeshall, N.D. *et al*, *J.A.C.S.*, 1949, **71**, 3150 (*uv*)

6-*tert*-Butyl-3,4-dimethylphenol B-1-00419

2-(1,1-Dimethylethyl)-4,5-dimethylphenol, 9CI.
6-tert-Butyl-3,4-xylenol, 8CI

[1445-23-4]

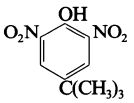
$C_{12}H_{18}O$ M 178.2
Fp 46-47°. Bp 258.5°, Bp_{10} 127°. n_D^{20} 1.5222.
Propanoyl: [121194-59-0].
$C_{15}H_{22}O_2$ M 234.3 Liq. Bp_{11} 147°.

McKinley, J.B. *et al*, *Ind. Eng. Chem., Anal. Ed.*, 1944, **16**, 304 (*deriv*)
Pardee, W.A. *et al*, *Ind. Eng. Chem.*, 1944, **36**, 595 (*synth, props*)
Martin, R. *et al*, *Synthesis*, 1989, 25 (*propanoyl*)

4-*tert*-Butyl-2,6-dinitrophenol B-1-00420

4-(1,1-Dimethylethyl)-2,6-dinitrophenol, 9CI

[4097-49-8]



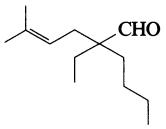
$C_{10}H_{12}N_2O_5$ M 240.2
Used in orange hair dyes. Mp 97-98° (85°).
Na salt: Yellow cryst.
Ca salt (2:1): Pale yellow cryst.
Guanidium salt: Brick red cryst. Mp 285°.
Me ether: 5-tert-Butyl-2-methoxy-1,3-dinitrobenzene
$C_{11}H_{14}N_2O_5$ M 254.2 Yellow leaflets (EtOH). Mp 101-102°.
Et ether: 5-tert-Butyl-2-ethoxy-1,3-dinitrobenzene
$C_{12}H_{16}N_2O_5$ M 268.2 Yellow leaflets. Mp 95-96°.

Henry, T.A. *et al*, *J.C.S.*, 1926, 2432 (*synth*)
Schaaf, O.H., *J. Prakt. Chem.*, 1932, **133**, 173 (*synth*)
U.S. Pat., 2 192 197, (1936); *CA*, **34**, 4528d (*synth*)
Dutton, G.S. *et al*, *Can. J. Chem.*, 1953, **31**, 685 (*derivs*)
Hall, R.C. *et al*, *J. Agric. Food Chem.*, 1972, **20**, 546 (*synth*)
Ger. Pat., 3 825 163, (1990); *CA*, **113**, 217777v (*use*)

2-Butyl-2-ethyl-5-methyl-4-hexenal B-1-00421

Irisal

[42023-59-6]



$C_{13}H_{24}O$ M 196.3
Perfumery compd.

Dieti, H.K. *et al*, *Tet. Lett.*, 1973, 1273 (*synth*)

2-*tert*-Butylfuran B-1-00422

2-(1,1-Dimethylethyl)furan, 9CI

[7040-43-9]

$C_8H_{12}O$ M 124.1
Liq. Bp 120°.

Magi, M. *et al*, *Org. Magn. Reson.*, 1977, **9**, 297 (*cmr*)
Fitzpatrick, J.E. *et al*, *Synth. Commun.*, 1982, **12**, 489 (*synth, pmr*)
Gribble, G.W. *et al*, *Magn. Reson. Chem.*, 1991, **29**, 422 (*synth, ir, pmr*)

3-*tert*-Butylfuran B-1-00423

3-(1,1-Dimethylethyl)furan

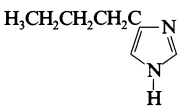
[7040-42-8]

$C_8H_{12}O$ M 124.1
Liq. Bp 123.5-124°, Bp_{60} 59-64°.

Shiukin, N.I. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1967, 1618; *CA*, **68**, 95607u (*synth, ir, pmr*)
Miller, D. *et al*, *J.C.S.(C)*, 1969, 12 (*synth, ir, pmr*)
Kiewiet, A. *et al*, *Org. Magn. Reson.*, 1974, **6**, 461 (*cmr*)

4-Butyl-1*H*-imidazole B-1-00424

[146953-86-8]

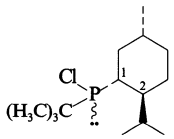


$C_7H_{12}N_2$ M 124.1
Waxy solid. $Bp_{0.1}$ 110-115°.

Keenan, R.M. *et al*, *J. Med. Chem.*, 1993, **36**, 1880 (*synth, pmr*)

tert-Butyl(2-isopropyl-5-methylcyclohexyl)phosphinous chloride, 8CI B-1-00425

(1,1-Dimethylethyl)[5-methyl-2-(1-methylethyl)cyclohexyl]phosphinous chloride, 9CI



$C_{14}H_{28}ClP$ M 262.8

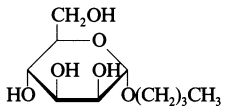
(***1R,2S,5R*)-*form*** [92808-59-8]

tert-*Butylmenthylphosphinous chloride.* tert-*Butylchloromenthylphosphine*
Liq. $Bp_{0.9}$ 118°. Phosphorus epimers not recognisable spectroscopically because of rapid halogen exchange.

[104012-57-9, 104012-58-0]

Brandos, H. *et al, Z. Naturforsch., B,* 1984, **39**, 1139 (*synth*)
Boese, R. *et al, Phosphorus Sulfur Relat. Elem.,* 1985, **25**, 103 (*synth, pmr, cmr, P-31 nmr*)
Hägele, G. *et al, J.C.S. Dalton,* 1987, 795 (*synth, pmr, cmr, P-31 nmr*)

Butyl mannoside B-1-00426



α-D-Pyranose-*form*

$C_{10}H_{20}O_6$ M 236.2

α-D-Pyranose-form [146453-36-3]
Constit. of the rhizomes of *Acanthopanax obovatus.* $[\alpha]_D^{20}$ −128.4 (c, 1.6 in MeOH).

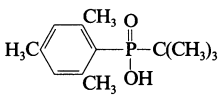
2,3,4,6-Tetrabenzoyl: [146399-93-1].
$C_{38}H_{36}O_{10}$ M 652.6 Syrup. $[\alpha]_D^{20}$ −16.7 (c, 0.6 in CH_2Cl_2).

β-D-Pyranose-form [143289-25-2]
Syrup. $[\alpha]_D^{20}$ −26.2 (c, 0.7 in H_2O).

Meldal, M. *et al, Carbohydr. Res.,* 1992, **235**, 115 (α-D-pyr, tetrabenzoyl, pmr, cmr)
Taubken, N. *et al, Synthesis,* 1992, 517 (β-D-pyr, pmr, cmr)
Taubken, N. *et al, J. Carbohydr. Chem.,* 1993, **12**, 651; 1994, **13**, 343 (β-D-pyr, pmr, cmr)
Si, J. *et al, Zhiwu Xuebao,* 1993, **35**, 483 (*isol*)

tert-Butylmesitylphosphinic acid B-1-00427

(*1,1-Dimethylethyl*)(*2,4,6-trimethylphenyl*) *phosphinic acid*



$C_{13}H_{21}O_2P$ M 240.2

Chloride: [147050-17-7].
$C_{13}H_{20}ClOP$ M 258.7 Cryst. (petrol). Mp 90.5-92.5°.

Amide: [147050-19-9].
$C_{13}H_{22}NOP$ M 239.2 Cryst. (toluene/petrol). Mp 157-158.5°.

Azide: [137248-25-0].
$C_{13}H_{20}N_3OP$ M 265.2 Cryst. Mp 46-48°. $Bp_{0.6}$ 140° (oven).

Harger, M.J.P. *et al, J.C.S. Perkin 1,* 1993, 227 (*synth, ms, ir, P-31 nmr*)

Butyl methyl disulfide, 9CI B-1-00428

[60779-24-0]

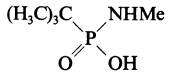
$H_3CCH_2CH_2CH_2—S—S—Me$

$C_5H_{12}S_2$ M 136.2
Liq. Bp_{10} 58°. n_D^{24} 1.5008.

Armitage, D.A. *et al, J.C.S. Perkin 1,* 1972, 680 (*synth*)
Zwanenburg, B. *et al, Tetrahedron,* 1979, **35**, 169 (*synth, pmr*)
Metzner, P. *et al, Synthesis,* 1994, 761 (*synth, pmr, cmr, ms*)

P-tert-Butyl-*N*-methylphosphonamidic acid B-1-00429

P-(*1,1-Dimethylethyl*)-N-*methylphosphonamidic acid*



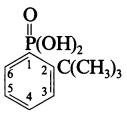
$C_5H_{14}NO_2P$ M 151.1

Me ester: [85656-10-6]. *Methyl* P-tert-*butyl*-N-*methylphosphonamidate*
$C_6H_{16}NO_2P$ M 165.1 Solid with low Mp. Bp_1 128-134° (oven).

Harger, M.J.P. *et al, Tetrahedron,* 1982, **38**, 3073 (*synth, ir, pmr*)

(2-*tert*-Butylphenyl) phosphonic acid, 8CI B-1-00430

[*2-(1,1-Dimethylethyl)phenyl*]*phosphonic acid, 9CI*



$C_{10}H_{15}O_3P$ M 214.2
Esters have yet only been synth. in isomer mixtures.

[72596-38-4, 124772-21-0]

Ohmori, H. *et al, J.C.S. Perkin 1,* 1979, 2023.
Romakhin, A.S. *et al, Electrochim. Acta,* 1989, **34**, 1417.

(3-*tert*-Butylphenyl) phosphonic acid, 8CI B-1-00431

[*3-(1,1-Dimethylethyl)phenyl*]*phosphonic acid, 9CI*

$C_{10}H_{15}O_3P$ M 214.2
Esters have yet only been synth. in isomer mixts.

[124772-18-5, 124772-25-4]

Romakhin, A.S. *et al, Electrochim. Acta,* 1989, **34**, 1417.

(4-*tert*-Butylphenyl) phosphonic acid, 8CI B-1-00432

[*4-(1,1-Dimethylethyl)phenyl*]*phosphonic acid*

[16839-07-9]

$C_{10}H_{15}O_3P$ M 214.2
Cryst. (H_2O). Mp 193-194°.

Di-Et ester: [72596-31-7]. *Diethyl* (*4*-tert-*butylphenyl)phosphonate*
$C_{14}H_{23}O_3P$ M 270.3 Liq. $Bp_{0.4}$ 142-143°.

[100134-03-0]

Romakhin, A.S. *et al, Electrochim. Acta,* 1989, **34**, 1417.
Katritzky, A.R. *et al, Org. Prep. Proced. Int.,* 1990, **22**, 209 (*synth, pmr, cmr*)
Yuan, C. *et al, Synthesis,* 1990, 140 (*synth, P-31 nmr*)
Hu, W. *et al, Chin. Chem. Lett.,* 1992, **3**, 579 (*P-31 nmr*)
Yuan, C. *et al, Heteroat. Chem.,* 1993, **4**, 23 (*P-31 nmr*)

tert-Butyl phenyl sulfide B-1-00433

[(*1,1-Dimethylethyl*)*thio*]*benzene, 9CI. 2-Methyl-2-(phenylthio)propane*

[3019-19-0]

$(H_3C)_3CSPh$

$C_{10}H_{14}S$ M 166.2
d_4^{20} 0.990. Bp_{10} 79-80°. n_D^{20} 1.5335.

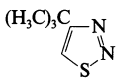
S,S-*Dioxide:* [4170-72-3]. tert-*Butyl phenyl sulfone*
$C_{10}H_{14}O_2S$ M 198.2 Needles. Mp 98-99°.

Ipatieff, V.N. *et al, J.A.C.S.,* 1938, **60**, 2731 (*synth*)
Iwao, M. *et al, J.O.C.,* 1989, **54**, 24 (*sulfone*)
Clayden, J. *et al, J.C.S. Perkin 1,* 1995, 7 (*synth*)

4-*tert*-Butyl-1,2,3-thiadiazole B-1-00434

4-(1,1-Dimethylethyl)-1,2,3-thiadiazole, 9CI

[40753-16-0]

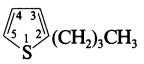


$C_6H_{10}N_2S$ M 142.2
Cryst. Mp 23°.

Seybold, G. *et al, Chem. Ber.,* 1977, **110**, 1225 (*synth*)
L'abbé, G. *et al, Bull. Soc. Chim. Belg.,* 1991, **100**, 623 (*cmr*)
L'abbé, G. *et al, J. Het. Chem.,* 1993, **30**, 301 (*N-15 nmr*)

2-Butylthiophene, 9CI B-1-00435

[1455-20-5]



$C_8H_{12}S$ M 140.2
Liq. d_4^{20} 0.9537. Bp 182-184°, Bp_{18} 97°. n_D^{20} 1.5004.

Pines, H. *et al, J.A.C.S.,* 1951, **73**, 5173 (*synth*)
Cagniant, P. *et al, Bull. Soc. Chim. Fr.,* 1955, 359 (*synth*)
Grey, T.F. *et al, J.C.S.,* 1960, 1502 (*synth*)
Suzuki, A. *et al, Bull. Soc. Chim. Fr.,* 1979, **52**, 1865 (*synth, ir, pmr*)

3-Butylthiophene, 9CI B-1-00436

[34722-01-5]

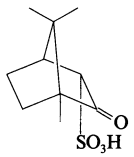
$C_8H_{12}S$ M 140.2
Liq. Bp_{739} 176-178°, Bp_{15} 85°. n_D^{20} 1.5114.

Wynberg, H. *et al, J.A.C.S.,* 1957, **79**, 1972 (*synth*)
Suzuki, A. *et al, Bull. Chem. Soc. Jpn.,* 1981, **54**, 1587 (*synth, ir, pmr*)
Zimmer, H. *et al, Synth. Commun.,* 1986, **16**, 689 (*synth, pmr*)
Budzikiewicz, H. *et al, Org. Mass Spectrom.,* 1994, **29**, 432 (*ms*)
Kirsch, G. *et al, Synth. Commun.,* 1994, **24**, 1721 (*synth, pmr*)

C

Camphor-3-sulfonic acid C-1-00001

4,7,7-Trimethyl-3-oxobicyclo[2.2.1]heptane-2-sulfonic acid, 9CI. 2-Oxo-3-bornanesulfonic acid, 8CI. Camphor-α-sulfonic acid



$C_{10}H_{16}O_4S$ M 232.3

(1RS,3SR)-form [22555-64-2]
(±)-endo-*form*
Mp 250° dec. (as Na salt).

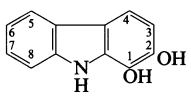
Chloride: [122437-11-0].
$C_{10}H_{15}ClO_3S$ M 250.7 Mp 45-48°.

[46365-22-4, 50894-65-0, 122518-20-1]

Cremlyn, R.J. *et al, Phosphorus Sulfur Relat. Elem.*, 1988, **39**, 165 (*synth, bibl*)

9*H*-Carbazole-1,2-diol C-1-00002

1,2-Dihydroxycarbazole



$C_{12}H_9NO_2$ M 199.2

Di-Me ether: 1,2-Dimethoxycarbazole
$C_{14}H_{13}NO_2$ M 227.2 Cryst. (EtOH). Mp 134°.

Loeffler, A. *et al, Nature (London)*, 1953, **172**, 820 (*synth, deriv*)

9*H*-Carbazole-1,4-diol, 9CI C-1-00003

1,4-Dihydroxycarbazole

$C_{12}H_9NO_2$ M 199.2

Di-Me ether: [100866-46-4]. *1,4-Dimethoxycarbazole, 9CI*
$C_{14}H_{13}NO_2$ M 227.2 Cryst. (EtOH aq.). Mp 111.5-113°.

Blackhall, A. *et al, J.C.S.*, 1954, 3916 (*synth, deriv*)
Smith, P.A.S. *et al, J.O.C.*, 1958, **23**, 524 (*synth, deriv*)
Parrick, J. *et al, J. Chem. Res., Synop.*, 1990, 1 (*synth, deriv*)

9*H*-Carbazole-2,7-diol, 9CI C-1-00004

2,7-Dihydroxycarbazole

$C_{12}H_9NO_2$ M 199.2

Di-Me ether: [61822-18-2]. *2,7-Dimethoxycarbazole, 9CI*
$C_{14}H_{13}NO_2$ M 227.2 Mp 272°.

Raj, K. *et al, Indian J. Chem., Sect. B*, 1976, **14**, 371.
Zelent, B. *et al, J. Photochem. Photobiol., A*, 1991, **56**, 165.

9*H*-Carbazole-3,6-diol C-1-00005

3,6-Dihydroxycarbazole

[15773-73-6]

$C_{12}H_9NO_2$ M 199.2
Mp >300°.

Di-Ac: [15773-75-8].
$C_{16}H_{13}NO_4$ M 283.2 Mp 212-214°.

Di-Me ether: 3,6-Dimethoxycarbazole
$C_{14}H_{13}NO_2$ M 227.2 Needles. Mp 102-104°, Mp 178-180°.

Stepanova, L.A. *et al, CA*, 1967, **67**, 73475b (*synth*)
Hsieh, B.R. *et al, Macromolecules*, 1986, **19**, 516 (*di-Me ether*)

3-[(Carboxymethyl)thio] propanoic acid, 9CI C-1-00006

Danosteine, *INN. 3-Thiahexanedioic acid*

[4938-00-5]

$HOOCCH_2SCH_2CH_2COOH$

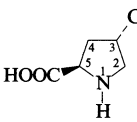
$C_5H_8O_4S$ M 164.1
Mucolytic agent. Reduces respiratory inflammation. Plates (C_6H_6). Mp 94°.

S-*Benzylthiouronium salt:* Cryst. (EtOH). Mp 156-157°.

Larsson, E. *et al, Ber.*, 1934, **67**, 757 (*synth*)
Schoeberl, A. *et al, Annalen*, 1956, **599**, 140 (*synth*)
Challenger, F. *et al, J.C.S.*, 1959, 61 (*synth*)
Laing, D.K. *et al, J.C.S. Dalton*, 1975, 2297 (*synth*)
Ger. Pat., 2 548 669, (1976) (*Joullie Internat*); *CA*, **85**, 104202 (*pharmacol*)
Gachon, F. *et al, Drug Metab. Dispos.*, 1988, **16**, 853 (*metab*)

5-Carboxy-3-pyrrolidineacetic acid, 9CI C-1-00007

4-(Carboxymethyl)-2-pyrrolidinecarboxylic acid. 4-(Carboxymethyl)proline



(*3R,5R*)-*form*

$C_7H_{11}NO_4$ M 173.1

(3R,5R)-form
(+)-trans-*form*
Solid. Mp 224-225°. $[\alpha]_D^{22}$ +66.8 (c, 0.5 in H_2O).

(3R,5S)-form
(−)-cis-*form*
Solid. Mp 234-235°. $[\alpha]_D^{22}$ −33.4 (c, 0.35 in H_2O).

(3S,5R)-form
(+)-cis-*form*
Solid. Mp 232-233°. $[\alpha]_D^{22}$ +34.2 (c, 0.5 in H_2O).

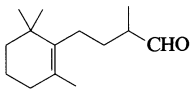
(3S,5S)-form [147235-94-7]
(−)-trans-*form*
Solid. Mp 228-229°. $[\alpha]_D^{22}$ −69 (c, 0.5 in H_2O) (−66.5).

Langlois, N. *et al, Tet. Lett.*, 1993, **34**, 2477 (*synth, pmr*)
Pellicciari, R. *et al, J.C.S. Perkin 1*, 1995, 1251 (*synth, pmr, cmr*)

Cetonal ™ C-1-00008

α,2,6,6-Tetramethyl-1-cyclohexene-1-butanal, 9CI. 2-Methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)butanal. Luciferin aldehyde

[84518-22-9]



$C_{14}H_{24}O$ M 208.3
Used in perfumery as blending agent.

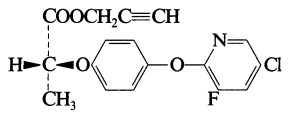
(±)-***form*** [28058-97-1]
Liq. with powerful woody-orris odour. Bp_2 90-100°, $Bp_{1.6}$ 93.5°. n_D^{21} 1.4821.

Fracheboud, M.G. *et al, Tet. Lett.*, 1969, 3951.
Nakatsubo, F. *et al, Tet. Lett.*, 1970, 381.
Ireland, R.E. *et al, J.O.C.*, 1971, **36**, 1195 (*synth*)
Kawanobe, T. *et al, Agric. Biol. Chem.*, 1986, **50**, 1475.
Japan. Pat., 61 254 516, (1986); *CA*, **106**, 8999k.
Weyersahl, P. *et al, Annalen*, 1988, **6**, 507 (*synth, ir, pmr, cmr*)

CGA 184927 C-1-00009

2-Propynyl 2-[4-[(5-chloro-3-fluoro-2-pyridinyl)oxy]phenoxy]propanoate, 9CI

[105511-96-4]



$C_{17}H_{13}ClFNO_4$ M 349.7

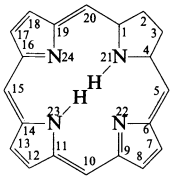
(R)-form [105512-06-9]
Herbicide. Inhibits lipid biosynth. Cryst. (EtOH). Mp 59.3° (55-56°).
▶ LD_{50} (rat, orl) 1829 mg/kg.

Eur. Pat., 248 968, (1987); *CA*, **108**, 204504 (*synth, use*)
Cornes, D.W. *et al, Brighton Crop Prot. Conf. Pests Dis.*, 1989, 71, 729 (*use*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A1256.

Chlorin C-1-00010

2,3-Dihydro-21H,23H-porphine, 9CI, 8CI

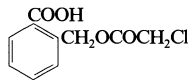
[2683-84-3]



$C_{20}H_{16}N_4$ M 312.3

Eisner, U. *et al, J.C.S.*, 1955, 3742 (*synth, uv*)
Renge, I., *J. Phys. Chem.*, 1993, **97**, 6582 (*uv*)
Listead, R.D. *et al, Spec. Publ. - Chem. Soc.*, 1995, **3**, 83 (*rev, synth, uv*)

2-(Chloroacetoxymethyl) benzoic acid C-1-00011



$C_{10}H_9ClO_4$ M 228.6
Protecting group for carbohydrates.

Chloride:
$C_{10}H_8Cl_2O_3$ M 247.0 No phys. props. reported.

Ziegler, T. *et al*, *Annalen*, 1994, 659.

2-Chlorobenzenemethanethiol, C-1-00012

9CI

2-Chlorobenzyl mercaptan. 2-Chloro-α-mercaptotoluene. o-Chloro-α-toluenethiol

[39718-00-8]

C_7H_7ClS M 158.6
Liq. Bp_{25} 120-121°, Bp_{13} 100-104°. n_D^{28} 1.5650. n_D^{20} 1.5904.

S-*(3,5-Dinitrobenzoyl):* Yellow cryst. Mp 112.5-113.5°.

S-*Me:* [57984-15-3]. *1-Chloro-2-[(methylthio) methyl]benzene, 9CI. 2-Chlorobenzyl methyl sulfide*
C_8H_9ClS M 172.6 Liq. Bp_{20} 123-124°, $Bp_{0.1}$ 52-62°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1091A.
Speroni, G. *et al*, *Gazz. Chim. Ital.*, 1940, **70**, 472 (*synth*)
Boenigk, J.W. *et al*, *J. Am. Pharm. Assoc.*, 1949, **38**, 357 (*synth*)
Lewis, T.R. *et al*, *J.A.C.S.*, 1951, **73**, 2109 (*synth*)
Tamura, Y. *et al*, *Synthesis*, 1975, 641 (*S-Me, synth*)

3-Chlorobenzenemethanethiol, C-1-00013

9CI

3-Chlorobenzyl mercaptan. m-*Chloro-α-toluenethiol, 8CI*

[25697-57-8]

C_7H_7ClS M 158.6
Liq. Bp_{19} 118°. n_D^{27} 1.5830.

S-*Me:* [35657-16-0]. *1-Chloro-3-[(methylthio) methyl]benzene, 9CI. 3-Chlorobenzyl methyl sulfide*
C_8H_9ClS M 172.6 Liq. Bp_{13} 117-118°.

Lombardino, J.G. *et al*, *J. Med. Chem.*, 1970, **13**, 206 (*synth*)

4-Chlorobenzenemethanethiol, C-1-00014

9CI

p-*Chloro-α-toluenethiol, 8CI. 4-Chlorobenzyl mercaptan. 1-Chloro-4-(mercaptomethyl) benzene. 4-Chloro-α-mercaptotoluene*

[6258-66-8]

C_7H_7ClS M 158.6
Liq. d 1.20. Mp 19-20°. Bp_{17} 113-114°, Bp_{10} 105°, $Bp_{0.4}$ 66-67°. n_D^{20} 1.5893. Stench.

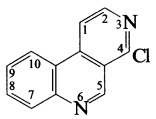
Na salt: [43170-85-0].
Solid.

S-*(3,5-Dinitrobenzoyl):* Yellow cryst. Mp 153.5-155°.

S-*Me:* [5925-82-6]. *1-Chloro-4-[(methylthio) methyl]benzene, 9CI. 4-Chlorobenzyl methyl sulfide*
C_8H_9ClS M 172.6 Liq. Bp_2 76-77°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1095A.
Aldrich Library of NMR Spectra, 2nd edn., **1**, 986A.
Lewis, T.R. *et al*, *J.A.C.S.*, 1951, **73**, 2109 (*synth*)
Kula, M. *et al*, *Can. J. Chem.*, 1956, **34**, 1093 (*synth*)
Molina, P. *et al*, *Synthesis*, 1982, 472 (*synth*)
Olah, G.A. *et al*, *Synthesis*, 1994, 277 (*S-Me, synth*)

4-Chlorobenzo[*c*][2,7] naphthyridine C-1-00015



$C_{12}H_7ClN_2$ M 214.6
Cryst. (Et_2O/cyclohexane). Mp 176°.

Cochennec, C. *et al*, *J.C.S. Perkin 1*, 1995, 979 (*synth, ir, pmr*)

6-Chloro-2*H*-1-benzopyran, C-1-00016

9CI, 8CI

*6-Chloro-2*H*-chromene*

[16336-27-9]

C_9H_7ClO M 166.6
Oil. $Bp_{14.5}$ 120°, Bp_1 68.5°. n_D^{20} 1.5995.

Maitte, P., *Ann. Chim. (Paris)*, 1954, **9**, 431 (*synth*)
Iwai, I. *et al*, *Chem. Pharm. Bull.*, 1963, **11**, 1042 (*synth, uv*)
Canalini, G. *et al*, *Ann. Chim. (Rome)*, 1967, **57**, 1045 (*synth, uv, pmr*)
Andreev, N.A. *et al*, *Zh. Org. Khim.*, 1984, **20**, 369; *J. Org. Chem. USSR (Engl. Transl.)*, 1984, **20**, 331 (*synth, pmr, ir*)

7-Chloro-2*H*-1-benzopyran, C-1-00017

8CI

*7-Chloro-2*H*-chromene*

[18385-91-6]

C_9H_7ClO M 166.6
Oil. $Bp_{0.4}$ 84-85°. n_D^{23} 1.6029.

Iwai, I. *et al*, *Chem. Pharm. Bull.*, 1963, **11**, 1042 (*synth, uv*)
Canalini, G. *et al*, *Ann. Chim. (Rome)*, 1967, **57**, 1045 (*synth, uv, pmr*)

8-Chloro-2*H*-1-benzopyran, C-1-00018

9CI, 8CI

*8-Chloro-2*H*-chromene*

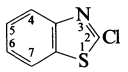
[42969-79-9]

C_9H_7ClO M 166.6
Oil. Bp_{12} 130°, $Bp_{1.5}$ 85.5°. n_D^{20} 1.6005.

Iwai, I. *et al*, *Chem. Pharm. Bull.*, 1963, **11**, 1042 (*synth, uv*)
Šarčević, N. *et al*, *Helv. Chim. Acta*, 1973, **56**, 92 (*synth, ir, uv, pmr, ms*)
Andreev, N.A. *et al*, *Zh. Org. Khim.*, 1984, **20**, 369; *J. Org. Chem. USSR (Engl. Transl.)*, 1984, **20**, 331 (*synth, pmr, ir*)

2-Chlorobenzothiazole C-1-00019

[615-20-3]



C_7H_4ClNS M 169.6
Liq. d_4^{20} 1.30. Mp 21-23°. Bp_{30} 141°, Bp_{21} 132-134°, Bp_2 70-73°. n_D^{20} 1.6380.

▶ DL3150000.

N-*Me:* see *2-Chloro-3-methylbenzothiazolium(1+), C-0-01997*

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1511D.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 574D.
Hofmann, A.F., *Ber.*, 1880, **13**, 9.
Davidovics, G. *et al*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1974, **71**, 659 (*ir, Raman*)
Sawhney, S.N. *et al*, *J.O.C.*, 1979, **44**, 1136 (*cmr*)
Czech. Pat., 233 447, (1983); *CA*, **106**, 196439 (*synth*)
Shibata, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1992, **65**, 3163 (*synth, ir*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 6th edn., Van Nostrand Reinhold, 1984, 683.

4-Chlorobenzothiazole C-1-00020

[3048-45-1]

C_7H_4ClNS M 169.6
Solid (pentane). Mp 57°.

Taddei, F. *et al*, *Gazz. Chim. Ital.*, 1965, **95**, 499 (*synth, pmr*)

5-Chlorobenzothiazole, 9CI C-1-00021

[2786-51-8]

C_7H_4ClNS M 169.6
Cryst. (EtOH). Mp 106°.

Lankelma, H.P. *et al*, *J.A.C.S.*, 1931, **53**, 2654 (*synth*)
Metzger, J. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 2857 (*synth*)
Taddei, F. *et al*, *Gazz. Chim. Ital.*, 1965, **95**, 499 (*pmr*)

6-Chlorobenzothiazole, 9CI C-1-00022

[2942-10-1]

C_7H_4ClNS M 169.6
Cryst. Mp 41°. Bp_2 111°.

Picrate: Bright yellow solid. Mp 136°.

Boggust, W.A. *et al*, *J.C.S.*, 1949, 355 (*synth*)
Takahashi, T. *et al*, *Yakugaku Zasshi*, 1960, **80**, 260; *CA*, **54**, 13103g (*synth*)
Taddei, F. *et al*, *Gazz. Chim. Ital.*, 1965, **95**, 499 (*pmr, synth*)
Sawhney, S.N. *et al*, *J.O.C.*, 1979, **44**, 1136 (*cmr*)

7-Chlorobenzothiazole C-1-00023

C_7H_4ClNS M 169.6
Solid (EtOH aq.). Mp 66°.

Taddei, F. *et al*, *Gazz. Chim. Ital.*, 1965, **95**, 499 (*synth, pmr*)

α-Chlorobenzylphosphonic acid C-1-00024

(Chlorophenylmethyl)phosphonic acid

$PhCHClP(O)(OH)_2$

$C_7H_8ClO_3P$ M 206.5

(±)-*form*

Di-Me ester: Dimethyl (α-chlorobenzyl) phosphonate. Dimethyl (chlorophenylmethyl)phosphonate
$C_9H_{12}ClO_3P$ M 234.6 Liq. $Bp_{0.07}$ 105°. n_D^{25} 1.5276.

Di-Et ester: Diethyl (α-chlorobenzyl) phosphonate. Diethyl (chlorophenylmethyl) phosphonate
$C_{11}H_{16}ClO_3P$ M 262.6 Liq. $Bp_{0.4}$ 118-120°. n_D^{20} 1.5116.

Dichloride: see *(Chlorophenylmethyl) phosphonic dichloride, C-1-00153*
[16965-75-6, 53378-80-6]

Seyforth, D. *et al, J.O.C.*, 1971, **36**, 1379 (*synth, ir, pmr*)
Petrova, J. *et al, Synthesis*, 1975, 658 (*ester, synth*)
Gajda, T., *Synthesis*, 1990, 717 (*di-Et ester, synth, ir, pmr, P-31 nmr*)

3-Chlorobicyclo[1.1.1]pentane-1-carboxylic acid, 9CI C-1-00025

[156329-73-6]

$C_6H_7ClO_2$ M 146.5
Cryst. by subl. Mp 165-165.5°.

Me ester: [156329-71-4].
$C_7H_9ClO_2$ M 160.6 Cryst. by subl. Mp 63-64°.

Della, E.W. *et al, J.O.C.*, 1994, **59**, 2986 (*synth, ir, pmr, cmr, ms*)

1-Chloro-2,2-bis(chloromethyl) butane, 9CI C-1-00026

1,1,1-Tris(chloromethyl)propane
[82925-88-0]

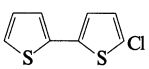
$H_3CCH_2C(CH_2Cl)_3$

$C_6H_{11}Cl_3$ M 189.5
Cryst. (MeOH). Mp 43-44°.

U.S. Pat., 2 441 595, (1948); *CA*, **42**, 7323f (*synth*)
Bolotov, A.A. *et al, Zh. Org. Khim.*, 1982, **18**, 2060; *CA*, **98**, 107261m (*synth*)

5-Chloro-2,2′-bithiophene, 9CI C-1-00027

5-Chloro-2,2′-bithienyl
[3339-85-3]



$C_8H_5ClS_2$ M 200.7
Oil. $Bp_{0.05}$ 55°.

Curtis, R.F. *et al, J.C.S.*, 1965, 5134 (*synth, uv*)

4-Chloro-2-buten-1-ol, 9CI C-1-00028

4-Chlorocrotyl alcohol
[7523-44-6]

$ClCH_2CH{=}CHCH_2OH$

C_4H_7ClO M 106.5

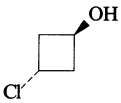
(*E*)-*form* [1775-39-9]
Liq. Bp_{10} 75-78°. n_D^{24} 1.4790.

Ac: [34414-28-3].
$C_6H_9ClO_2$ M 148.5 Liq. Bp_{17} 87°.

(*Z*)-*form* [1576-93-8]
Liq. Bp_{11} 79-81°. n_D^{25} 1.4838.

Colonge, J. *et al, Bull. Soc. Chim. Fr.*, 1955, 953 (*synth*)
Thomas, D.A. *et al, J.C.S.*, 1965, 2988 (*synth*)
Heasley, V.L. *et al, J.O.C.*, 1972, **37**, 2228 (*Ac*)
Imai, T. *et al, Synthesis*, 1993, 395 (*synth, pmr*)

3-Chlorocyclobutanol C-1-00029



(1*RS*,3*RS*)-*form*

C_4H_7ClO M 106.5
Bp_{20} 85-95°. *cis:trans* 60:40.

(*1RS,3RS*)-*form* [152713-95-6]
trans-*form*

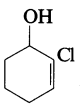
4-Methylbenzenesulfonyl: [26505-67-9].
Solid. Mp 39.0-39.5°.

(*1RS,3SR*)-*form* [152713-94-5]
cis-*form*
Liq. Sep. from *trans*-isomer by vpc.

4-Methylbenzenesulfonyl: [26505-66-8].
Cryst. (Et_2O/pentane). Mp 57.0-57.5°.

Wiberg, K.B. *et al, J.A.C.S.*, 1993, **115**, 1064S (*synth*)

2-Chloro-2-cyclohexen-1-ol C-1-00030



C_6H_9ClO M 132.5

(±)-*form* [109380-10-1]
Liq. Bp_{15} 86-87°. n_D^{20} 1.5088.

Ac: [109380-18-9].
$C_8H_{11}ClO_2$ M 174.6 Liq. Bp_{15} 106°. n_D^{20} 1.4804.

[67820-31-9]

Mousseron, M. *et al, Bull. Soc. Chim. Fr.*, 1950, 648 (*synth*)
Bergman, E., *J.O.C.*, 1963, **28**, 2210 (*synth, Ac*)
Domnin, N.A. *et al, Zh. Obshch. Khim.*, 1964, **34**, 2848; *J. Gen. Chem. USSR (Engl. Transl.)*, 1964, **34**, 2881 (*synth*)
Bentley, T.W. *et al, Annalen*, 1995, 599 (*synth, pmr, cmr*)

1-Chlorocyclooctene, 9CI C-1-00031

[1890-22-8]

$C_8H_{13}Cl$ M 144.6

(*E*)-*form* [86428-68-4]
cis-*form*
Oil. Bp_{31} 86-86.8°. n_D^{20} 1.4927.

Kohler, E.P. *et al, J.A.C.S.*, 1939, **61**, 1057 (*synth*)
Braude, E.A. *et al, J.C.S.*, 1957, 4711 (*synth, ir*)
Brown, A.B. *et al, Synth. Commun.*, 1995, **25**, 485 (*synth, ir, pmr, cmr*)

3-Chlorocyclooctene, 9CI C-1-00032

[24618-80-2]

$C_8H_{13}Cl$ M 144.6

(±)-(*Z*)-*form*
Liq. Bp_{13} 71-72°. n_D^{20} 1.4952.

[14796-70-4]

Henniger, P.W. *et al, Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1966, **85**, 1177 (*synth*)
Penman, K.G. *et al, J.C.S. Perkin 1*, 1991, 721 (*cmr*)

4-Chlorocyclooctene, 9CI C-1-00033

$C_8H_{13}Cl$ M 144.6

(±)-(*Z*)-*form*
Liq. Bp_{10} 67-69°. n_D^{20} 1.4965.

[14987-71-4]

Henniger, P.W. *et al, Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1966, **85**, 1177 (*synth*)
Andrejević, V. *et al, J. Serb. Chem. Soc.*, 1989, **54**, 325 (*ir, pmr, ms*)

5-Chlorocyclooctene, 9CI C-1-00034

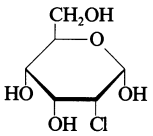
[1855-55-6]

$C_8H_{13}Cl$ M 144.6

(±)-(*Z*)-*form*
Oil. Bp_{10} 71-72°.

Ashby, E.C. *et al, J.O.C.*, 1986, **51**, 3598 (*synth, pmr*)
Bloodworth, A.J. *et al, J.C.S. Perkin 1*, 1990, 2957 (*synth, pmr, cmr, ms*)

2-Chloro-2-deoxyallose C-1-00035



α-D-Pyranose-*form*

$C_6H_{11}ClO_5$ M 198.6

α-D-Pyranose-form

Me glycoside: Methyl 2-chloro-2-deoxy-α-D-allopyranoside
$C_7H_{13}ClO_5$ M 212.6 Cryst. Mp 160-161°. $[\alpha]_D$ +111 (MeOH).

Me glycoside, 3,4-O-benzylidene (R-)*:* [35775-03-2].
$C_{14}H_{17}ClO_5$ M 300.7 Syrup. $[\alpha]_D^{20}$ +20 (c, 3.0 in $CHCl_3$).

Me glycoside, 4,6-O-benzylidene: [35775-02-1].
$C_{14}H_{17}ClO_5$ M 300.7 Cryst. Mp 102-103.5°. $[\alpha]_D$ +88.4 ($CHCl_3$).

Me glycoside, 4,6-O-benzylidene, 3-Me: [19685-18-8].
$C_{15}H_{19}ClO_5$ M 314.7 Cryst. (Me_2CO/Et_2O/petrol). Mp 121-122°. $[\alpha]_D$ +68 (c, 0.82 in $CHCl_3$).

Me glycoside, 3,4-O-isopropylidene:
$C_{10}H_{17}ClO_5$ M 252.6 Mp 60°. $[\alpha]_D$ +75.9 ($CHCl_3$).

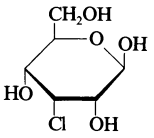
β-D-Pyranose-form

1,6-Anhydro, 3,4-di-Ac:
$C_{10}H_{13}ClO_6$ M 264.6 Cryst. Mp 90-91°. $[\alpha]_D$ −212 ($CHCl_3$).

Newth, F.H. *et al, J.C.S.*, 1947, 10 (*isopropylidene, β-D-deriv*)
Richards, G.N. *et al, J.C.S.*, 1956, 496 (*4,6-benzylidene*)

Hanessian, S. *et al*, *J.O.C.*, 1969, **34**, 2163 (*3-Me, pmr*)
Inch, T.D. *et al*, *Carbohydr. Res.*, 1972, **21**, 37 (*benzylidene*)

3-Chloro-3-deoxyallose C-1-00036


β-D-Pyranose-*form*

$C_6H_{11}ClO_5$ M 198.6

β-D-Pyranose-form

Me glycoside: [4991-00-8].
$C_7H_{13}ClO_5$ M 212.6 Syrup. $[\alpha]_D^{23}$ −49 (c, 1.0 in H_2O), $[\alpha]_D$ +51 (c, 1.0 in MeOH). Widely varying $[\alpha]_D$ values in the literature.

Me glycoside, 4,6-O-benzylidene: [4990-99-2].
$C_{14}H_{17}ClO_5$ M 300.7 Cryst. (Et_2O). Mp 132-133° (125.5-127°). $[\alpha]_D$ +50.5 (c, 1.0 in $CHCl_3$), $[\alpha]_D^{25}$ −47 (c, 1.02 in $CHCl_3$). Widely varying $[\alpha]_D$ values in the literature.

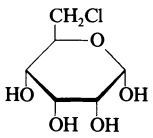
Me glycoside, 4,6-O-benzylidene (R-), *2-Ac:* [131474-43-6].
$C_{16}H_{19}ClO_6$ M 342.7 $[\alpha]_D$ −94 (c, 1.0 in CH_2Cl_2).

α-D-Furanose-form

1,2:5,6-Di-O-isopropylidene: [74925-18-1].
$C_{12}H_{19}ClO_5$ M 278.7 Cryst. Mp 52°. $[\alpha]_D^{22}$ +41 (c, 1.0 in $CHCl_3$).

Williams, E.H. *et al*, *Can. J. Chem.*, 1971, **49**, 796 (*β-Me gly, benzylidene*)
Arita, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 567 (*benzylidene*)
Szarek, W.A. *et al*, *Can. J. Chem.*, 1974, **52**, 3394 (*benzylidene, cmr*)
Kunz, H. *et al*, *Annalen*, 1982, 1245 (*diisopropylidene*)
Khan, R. *et al*, *Carbohydr. Res.*, 1990, **205**, 211 (*β-Me gly deriv, pmr, cmr, ms*)

6-Chloro-6-deoxyallose C-1-00037



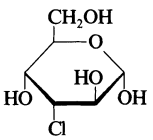
$C_6H_{11}ClO_5$ M 198.6

α-D-Pyranose-form

Me glycoside, 2,3-anhydro: [19685-17-7].
$C_7H_{11}ClO_4$ M 194.6 Cryst. (Et_2O/petrol). Mp 93-94°. $[\alpha]_D$ +155 (c, 0.59 in $CHCl_3$).

Hanessian, S. *et al*, *J.O.C.*, 1969, **34**, 2163 (*anhydro, pmr*)

3-Chloro-3-deoxyaltrose C-1-00038


α-D-Pyranose-*form*

$C_6H_{11}ClO_5$ M 198.6

α-D-Pyranose-form

Me glycoside:
$C_7H_{13}ClO_5$ M 212.6 Syrup. $[\alpha]_D^{20}$ +103.5 (c, 1.0 in EtOH).

Me glycoside, tri-Ac:
$C_{13}H_{19}ClO_8$ M 338.7 Cryst. (EtOH). Mp 98-99°. $[\alpha]_D^{20}$ +70.3 ($CHCl_3$), $[\alpha]_D^{20}$ +73 (c, 1.61 in $CHCl_3$).

Me glycoside, 4,6-O-benzylidene (R-): [131613-80-4].
$C_{14}H_{17}ClO_5$ M 300.7 Syrup.

Me glycoside, 4,6-O-benzylidene, 2-Ac:
$C_{16}H_{19}ClO_6$ M 342.7 Cryst. (EtOH). Mp 126°. $[\alpha]_D^{17}$ +90 (c, 1.89 in $CHCl_3$).

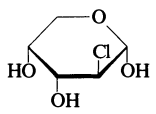
β-D-Pyranose-form

Me glycoside: Cryst. (EtOAc). Mp 128-129°. $[\alpha]_D^{20}$ −111.8 (c, 0.33 in EtOH).

1,6-Anhydro, 2,4-di-Ac:
$C_{10}H_{13}ClO_6$ M 264.6 Cryst. (EtOH). Mp 114-115°. $[\alpha]_D^{19}$ −202 (c, 0.91 in $CHCl_3$).

Newth, F.H. *et al*, *J.C.S.*, 1953, 989 (*α-Me-gly, β-Me gly, anhydro*)
Hughes, A.B. *et al*, *Aust. J. Chem.*, 1990, **43**, 1681 (*benzylidene, pmr*)

2-Chloro-2-deoxyarabinose C-1-00039


α-D-Pyranose-*form*

$C_5H_9ClO_4$ M 168.5

D-form

Mp 135°. $[\alpha]_D$ −126 (H_2O).

Diethyl dithioacetal:
$C_9H_{19}ClO_3S_2$ M 274.8 Mp 83° dec. $[\alpha]_D^{20}$ +67 (c, 2.0 in dioxan).

α-D-Pyranose-form

Me glycoside, 3,4-di-Ac:
$C_{10}H_{15}ClO_6$ M 266.6 Cryst. Mp 99-100°. $[\alpha]_D$ −59.6 ($CHCl_3$).

α-D-Furanose-form

Tri-Ac: [30589-74-3].
$C_{11}H_{15}ClO_7$ M 294.6 $Bp_{0.2}$ 135°. $[\alpha]_D^{20}$ +28.1 (c, 1.0 in $CHCl_3$).

Me glycoside: [55735-87-0]. *Methyl 2-chloro-2-deoxy-α-D-arabinofuranoside*
$C_6H_{11}ClO_4$ M 182.6 Syrup.

Me glycoside, 3,5-di-Ac: [55735-88-1].
$C_{10}H_{15}ClO_6$ M 266.6 Syrup. $Bp_{0.08}$ 100°. $[\alpha]_D^{20}$ +45.2 (c, 2.0 in $CHCl_3$).

Me glycoside, 3,5-dibenzyl: [55740-54-0].
$C_{20}H_{23}ClO_4$ M 362.8 Syrup.

Et glycoside, 3,5-di-Ac:
$C_{11}H_{17}ClO_6$ M 280.7 $Bp_{0.02}$ 87°. $[\alpha]_D^{20}$ +25 (c, 2.0 in $CHCl_3$).

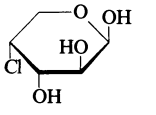
β-D-Furanose-form

Me glycoside: Methyl 2-chloro-2-deoxy-β-D-arabinofuranoside
$C_6H_{11}ClO_4$ M 182.6 Syrup. $[\alpha]_D^{20}$ −95.1 (c, 2.0 in H_2O).

Me glycoside, 3,5-di-Ac: Cryst. (C_6H_6/petrol). Mp 74-76°. $Bp_{0.2}$ 115-117°. $[\alpha]_D^{20}$ −122 (c, 2.0 in $CHCl_3$).

Vargha, L. *et al*, *Chem. Ber.*, 1963, **96**, 411 (D-form, α-Me pyr)
Kuszmann, J. *et al*, *Chem. Ber.*, 1963, **96**, 2327 (D-form deriv, Me β-D-fur, α-Et fur)
Ritzmann, G. *et al*, *Carbohydr. Res.*, 1975, **39**, 227 (*Me* α-D-fur)
Kuszmann, J. *et al*, *Carbohydr. Res.*, 1979, **14**, 415 (*tri-Ac*)
Ilicheva, I.A. *et al*, *Bioorg. Khim.*, 1989, **15**, 800; *Sov. J. Bioorg. Chem.* (*Engl. Transl.*), 1989, **15**, 428 (*conformn*)

4-Chloro-4-deoxyarabinose C-1-00040


β-D-Pyranose-*form*

$C_5H_9ClO_4$ M 168.5

β-D-Pyranose-form

Me glycoside:
$C_6H_{11}ClO_4$ M 182.6 Needles (EtOAc). Mp 152°. $[\alpha]_D$ +237 (c, 0.96 in MeOH).

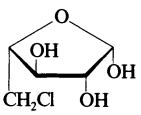
L-form

Cryst. (EtOH). Mp 150°. $[\alpha]_D$ +155 → 119 (equilib.) (c, 0.4 in H_2O).

Phenylosazone: Yellow cryst. (MeOH aq.). Mp 123° dec.

Jennings, H.J. *et al*, *Can. J. Chem.*, 1962, **40**, 1408 (*synth*, L-form, Me gly)
Barnett, J.E.G., *Adv. Carbohydr. Chem.*, 1967, **22**, 177 (*rev*)

5-Chloro-5-deoxyarabinose C-1-00041



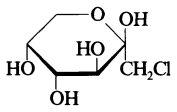
$C_5H_9ClO_4$ M 168.5

β-L-Furanose-form

1,2-O-Isopropylidene, 3-mesyl: [105953-27-3].
$C_9H_{15}ClO_6S$ M 286.7 Cryst. (diisopropyl ether). Mp 58-59°. $[\alpha]_D$ −4 (c, 0.50 in $CHCl_3$).

Hughes, N.A. *et al*, *J.C.S. Perkin 1*, 1986, 695 (*isopropylidene deriv, pmr*)

1-Chloro-1-deoxyfructose C-1-00042


β-D-Pyranose-*form*

$C_6H_{11}ClO_5$ M 198.6

D-form [32785-93-6]
Syrup. $[\alpha]_D^{22}$ −63 (c, 0.25 in H_2O), $[\alpha]_D$ −53.3 (c, 1.38 in H_2O).

Tetra-Ac:
$C_{14}H_{19}ClO_9$ M 366.7 Cryst. (Et_2O/petrol). Mp 77.5-78°. $[\alpha]_D$ +68 (c, 0.4 in $CHCl_3$).

β-D-Pyranose-form

2,3:4,5-Di-O-isopropylidene: [32785-90-3].
$C_{12}H_{19}ClO_5$ M 278.7 Cryst. (Et_2O/petrol). Mp 53-53.5°. $[\alpha]_D^{22}$ −29.5 (c, 0.19 in $CHCl_3$).

α-D-Furanose-form

Me glycoside: [82877-67-6]. *Methyl 1-chloro-1-deoxy-α-D-fructofuranoside*
$C_7H_{13}ClO_5$ M 212.6 Syrup. $[\alpha]_D^{25}$ +63.7 (MeOH).

Me glycoside, tri-Ac: [82877-49-4].
$C_{13}H_{19}ClO_8$ M 338.7 Cryst. ($CHCl_3$/hexane). Mp 73.5-74.5°. $[\alpha]_D^{25}$ + 113 ($CHCl_3$).

β-D-Furanose-form

2,3-O-Isopropylidene: [83032-07-9].
$C_9H_{15}ClO_5$ M 238.6 Cryst. ($CHCl_3$/hexane). Mp 94.5-95.5°. $[\alpha]_D^{25}$ +12.4 ($CHCl_3$).

Me glycoside: [82877-68-7]. *Methyl 1-chloro-1-deoxy-β-D-fructofuranoside*
$C_7H_{13}ClO_5$ M 212.6 Hygroscopic syrup. $[\alpha]_D^{25}$ −46.7 (MeOH).

Me glycoside, tri-Ac: [82877-56-3].
Syrup. $[\alpha]_D^{25}$ −30.7 ($CHCl_3$).

L-form

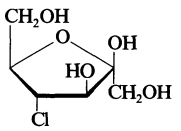
Tetra-Ac: [23261-13-4].
Cryst. (Et_2O/petrol). Mp 76-77°. $[\alpha]_D^{23}$ −68 (c, 4.0 in $CHCl_3$).

DL-form

Tetra-Ac: [23261-14-5].
Cryst. Mp 101°.

Wolfrom, M.L. *et al, J.A.C.S.*, 1942, **64**, 1701 (D-tetra-Ac)
Humphlett, W.J., *Carbohydr. Res.*, 1968, **7**, 43 (L-tetra-Ac, DL-tetra-Ac)
Haylock, C.R. *et al, Carbohydr. Res.*, 1971, **16**, 375 (*synth*, D-form, diisopropylidene)
Barnett, J.E.G. *et al, Carbohydr. Res.*, 1972, **25**, 511 (*synth*, D-form, diisopropylidene)
Guthrie, R.D. *et al, Aust. J. Chem.*, 1982, **35**, 1003 (*isopropylidene, α-Me fur deriv, β-Me fur deriv, pmr*)
Caldwell, G.W. *et al, Org. Mass Spectrom.*, 1989, **24**, 1051 (*ms*)

4-Chloro-4-deoxyfructose C-1-00043



β-D-Furanose-*form*

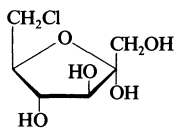
$C_6H_{11}ClO_5$ M 198.6

β-D-Furanose-form

2,3-O-Isopropylidene, 1,6-ditosyl: [82064-04-8].
$C_{23}H_{27}ClO_9S_2$ M 547.0 Mp 99-99.5°. $[\alpha]_D$ +20 (c, 1.0 in $CHCl_3$).

Guthrie, R.D. *et al, Carbohydr. Res.*, 1982, **103**, 1 (*isopropylidene, cmr*)

6-Chloro-6-deoxyfructose C-1-00044



α-D-Furanose-*form*

$C_6H_{11}ClO_5$ M 198.6

D-form [66451-66-9]
Potential use as a male contraceptive. Exhibits anti-fertility activity in male rats.

Tetra-Ac:
$C_{14}H_{19}ClO_9$ M 366.7 Cryst. Mp 108°. $[\alpha]_D$ +45.3 ($CHCl_3$).

α-D-Furanose-form

Me glycoside: [70836-64-5]. *Methyl 6-chloro-6-deoxy-α-D-fructofuranoside*
$C_7H_{13}ClO_5$ M 212.6 Cryst. (MeOH). Mp 71-73° (70.6-71.5°). $[\alpha]_D$ +40 (c, 0.5 in MeOH), $[\alpha]_D^{25}$ +47 (MeOH).

Me glycoside, 1-tosyl: [83031-91-8].
Syrup. $[\alpha]_D^{25}$ +23.1 ($CHCl_3$).

β-D-Furanose-form

2,3-O-Isopropylidene: [83032-10-4].
$C_9H_{15}ClO_5$ M 238.6 Mp 73-74°. $[\alpha]_D^{25}$ +4.9 ($CHCl_3$).

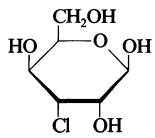
2,3-O-Isopropylidene, 1-tosyl: [82064-02-6].
Cryst. (MeOH). Mp 76°. $[\alpha]_D$ +17 (c, 1.0 in $CHCl_3$).

Me glycoside: [70836-65-6]. *Methyl-6-chloro-6-deoxy-β-D-fructofuranoside*
$C_7H_{13}ClO_5$ M 212.6 Cryst. (MeOH). Mp 98-99°. $[\alpha]_D^{25}$ −35 ($CHCl_3$).

Me glycoside, 1-tosyl: [83031-82-7].
Syrup. $[\alpha]_D^{25}$ −23.6 ($CHCl_3$).

Pacsu, E. *et al, J.A.C.S.*, 1933, **55**, 3018 (D-tetra-Ac)
Ford, W.C.L., *Clin. Androl.*, 1980, **5**, 123; *CA*, **96**, 174597x (*pharmacol*)
Guthrie, R.D. *et al, Aust. J. Chem.*, 1982, **35**, 1003, 1019 (*α-Me fur, α-Me fur derivs, β-Me fur, β-Me fur derivs, pmr*)
Guthrie, R.D. *et al, Carbohydr. Res.*, 1982, **103**, 1 (*β-Me fur tosyl, pmr, cmr, ms*)

3-Chloro-3-deoxygulose C-1-00045



β-D-Pyranose-*form*

$C_6H_{11}ClO_5$ M 198.6

α-D-Pyranose-form

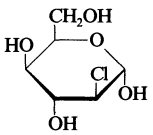
Me glycoside: [101947-68-6].
$C_7H_{13}ClO_5$ M 212.6 Prisms. Mp 142° dec. $[\alpha]_D^{24}$ +114.5 (c, 1.2 in H_2O).

β-D-Pyranose-form

Me glycoside, 4-(N,N-dimethylcarbamoyl), 2,6-di-Me: [84730-46-1].
$C_{12}H_{22}ClNO_6$ M 311.7 Prisms (diisopropyl ether/pentane). Mp 58-60°. $[\alpha]_D^{22}$ −65 ($CHCl_3$).

Buchanan, J.G., *J.C.S.*, 1958, 2511 (*α-Me pyr*)
Copeland, C. *et al, Aust. J. Chem.*, 1982, **35**, 2257 (*β-Me pyr deriv*)
Toufeili, I.A. *et al, Aust. J. Chem.*, 1985, **38**, 1425 (*α-Me pyr, cmr*)

2-Chloro-2-deoxyidose C-1-00046



$C_6H_{11}ClO_5$ M 198.6

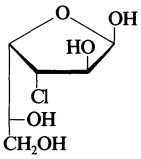
α-D-Pyranose-form

Me glycoside:
$C_7H_{13}ClO_5$ M 212.6 Cryst. Mp 124-126°. $[\alpha]_D$ +86.6 (H_2O).

Me glycoside, 4,6-O-benzylidene:
$C_{14}H_{17}ClO_5$ M 300.7 Cryst. Mp 166°. $[\alpha]_D$ +64.8 ($CHCl_3$).

Buchanan, J.G., *J.C.S.*, 1958, 995 (*α-Me gly, benzylidene*)

3-Chloro-3-deoxyidose C-1-00047



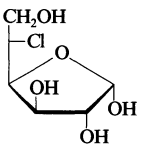
$C_6H_{11}ClO_5$ M 198.6

β-D-Furanose-form

1,2:5,6-Di-O-isopropylidene: [32785-97-0].
$C_{12}H_{19}ClO_5$ M 278.7 Cryst. (petrol). Mp 108.5-110°. $[\alpha]_D$ +24.7 (c, 0.65 in cyclohexane).

Haylock, C.R. *et al, Carbohydr. Res.*, 1971, **16**, 375 (*diisopropylidene, pmr*)

5-Chloro-5-deoxyidose C-1-00048



$C_6H_{11}ClO_5$ M 198.6

β-L-Furanose-form

1,2-O-Isopropylidene: [69465-26-5].
$C_9H_{15}ClO_5$ M 238.6 Cryst. (Et_2O/petrol). Mp 106-107°. $[\alpha]_D$ −31 (c, 0.5 in MeOH).

1,2-O-Isopropylidene, 6-benzoyl, 3-Ac: [118176-22-0].
$C_{18}H_{21}ClO_7$ M 384.8 Cryst. (Et_2O). Mp 143-144°. $[\alpha]_D$ −12 (c, 0.5 in CH_2Cl_2).

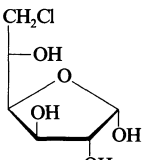
1,2-O-Isopropylidene, 3,6-dibenzoyl: [118176-23-1].
$C_{23}H_{23}ClO_7$ M 446.8 Cryst. (Et_2O/petrol). Mp 103-104°. $[\alpha]_D$ −43 (c, 0.3 in CH_2Cl_2).

1,2-O-Isopropylidene, 6-(methoxymethyl): [130619-46-4].
$C_{11}H_{19}ClO_6$ M 282.7 Syrup. $[\alpha]_D^{20}$ +1.6 (c, 3.1 in $CHCl_3$).

1,2:3,6-Di-O-isopropylidene: [82893-17-2].
$C_{12}H_{19}ClO_5$ M 278.7 Syrup. $[\alpha]_D^{22}$ +48.8 (c, 2.5 in $CHCl_3$).

Klemer, A. *et al, Carbohydr. Res.*, 1979, **68**, 391 (*isopropylidene*)
Kunz, H. *et al, Annalen*, 1982, 1245 (*diisopropylidene*)
Lee, C.K., *Carbohydr. Res.*, 1988, **177**, 247 (*isopropylidene, pmr*)
Dax, R. *et al, J. Carbohydr. Chem.*, 1990, **2**, 479 (*methoxymethyl*)

6-Chloro-6-deoxyidose C-1-00049



$C_6H_{11}ClO_5$ M 198.6

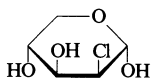
β-L-Furanose-form

1,2-O-Isopropylidene: [118176-24-2].
$C_9H_{15}ClO_5$ M 238.6 Cryst. (Et_2O/petrol). Mp 106-107°. $[\alpha]_D$ −31 (c, 0.5 in MeOH).

1,2-O-Isopropylidene, 5-benzoyl, 3-tosyl: [28642-60-6].
$C_{23}H_{25}ClO_8S$ M 496.9 Syrup. $[\alpha]_D^{25}$ +9 (c, 1.1 in $CHCl_3$).

Chalk, R.C. *et al, Carbohydr. Res.*, 1971, **20**, 151 (*isopropylidene, pmr, cmr*)
Lee, C.K., *Carbohydr. Res.*, 1988, **177**, 247 (*isopropylidene deriv*)

2-Chloro-2-deoxylyxose C-1-00050



α-D-Pyranose-*form*

$C_5H_9ClO_4$ M 168.5

α-D-Pyranose-form [29217-61-6]
Cryst. (Me_2CO/Et_2O). Mp 157-159°. $[\alpha]_D$ −0.5 → −15.5 (equilib.) (c, 1.03 in MeOH).

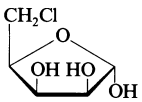
Me glycoside, di-Ac: [51385-06-9].
$C_{10}H_{15}ClO_6$ M 266.6 Syrup. $[\alpha]_D^{25}$ +8 (c, 1.71 in $CHCl_3$).

β-D-Pyranose-form

Me glycoside: [29217-60-5].
$C_6H_{11}ClO_4$ M 182.6 Syrup. $[\alpha]_D^{21}$ −96 (c, 1.3 in $CHCl_3$).

Jennings, H.J. *et al, Can. J. Chem.*, 1970, **48**, 1834 (*synth, β-Me pyr*)
Van Es, T., *J. S. Afr. Chem. Inst.*, 1973, **26**, 152 (*α-Me pyr deriv, pmr*)

5-Chloro-5-deoxylyxose C-1-00051



$C_5H_9ClO_4$ M 168.5

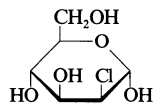
α-D-Furanose-form

Me glycoside:
$C_6H_{11}ClO_4$ M 182.6 Known as a cyclic phosphonate deriv.

[90213-32-4]

Koroteev, M.P. *et al, Zh. Obshch. Khim.*, 1984, **54**, 279; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1984, **54**, 245 (*Me gly deriv, pmr*)

2-Chloro-2-deoxymannose C-1-00052



α-D-Pyranose-*form*

$C_6H_{11}ClO_5$ M 198.6

α-D-Pyranose-form

3,4,6-Tri-Ac: [50603-56-0].
$C_{12}H_{17}ClO_8$ M 324.7 Amorph. $[\alpha]_D^{20}$ +19 (c, 2.5 in $CHCl_3$).

Tetra-Ac: [50603-57-1].
$C_{14}H_{19}ClO_9$ M 366.7 Cryst. (Et_2O/petrol). Mp 97°. $[\alpha]_D^{20}$ +6.8 (c, 0.9 in $CHCl_3$).

1-Benzoyl, tri-Ac: [23259-30-5].
$C_{19}H_{21}ClO_9$ M 428.8 Cryst. (EtOH). Mp 169-170°. $[\alpha]_D^{28}$ +79.3 (c, 0.52 in $CHCl_3$).

Me glycoside: [20512-21-4]. *Methyl 2-chloro-2-deoxy-α-D-mannopyranoside*
$C_7H_{13}ClO_5$ M 212.6 Syrup. $[\alpha]_D^{24}$ +81.1 (c, 0.95 in MeOH).

Me glycoside, tri-Ac: [22931-82-4].
$C_{13}H_{19}ClO_8$ M 338.7 Syrup. $[\alpha]_D^{24}$ +45.1 (c, 1.02 in $CHCl_3$), $[\alpha]_D^{23}$ +37.4 ($CHCl_3$).

Me glycoside, 4,6-O-benzylidene (R-)*:* [131564-58-4].
$C_{14}H_{17}ClO_5$ M 300.7 Cryst. (Et_2O/petrol). Mp 89°. $[\alpha]_D$ +39 (c, 1.0 in CH_2Cl_2).

Me glycoside, 4,6-O-benzylidene (R-), *3-benzoyl:* [131564-59-5].
$C_{21}H_{21}ClO_6$ M 404.8 Syrup. $[\alpha]_D$ +99.5 (c, 1.0 in $CHCl_3$).

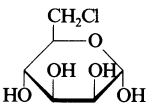
β-D-Pyranose-form

Me glycoside: [20513-88-6]. *Methyl 2-chloro-2-deoxy-β-D-mannopyranoside*
$C_7H_{13}ClO_5$ M 212.6 Plates (EtOAc). Mp 134-134.5°. $[\alpha]_D^{24}$ −78.6 (c, 1.05 in MeOH).

Me glycoside, tri-Ac: [20512-22-5].
Cryst. Mp 120.5-121°. $[\alpha]_D^{22.5}$ −86.9 ($CHCl_3$).

Igarashi, K. *et al, Tet. Lett.*, 1968, 755 (*α-Me gly, β-Me gly*)
Hall, L.D. *et al, Can. J. Chem.*, 1969, **47**, 379 (*1-benzoyl*)
Igarashi, K. *et al, J.O.C.*, 1970, **35**, 610 (*α-Me gly, β-Me gly*)
Boullanger, P. *et al, Bull. Soc. Chim. Fr.*, 1973, 2149 (*Ac derivs, pmr*)
Khan, R. *et al, Carbohydr. Res.*, 1990, **205**, 211 (*benzylidene deriv, pmr, cmr*)

6-Chloro-6-deoxymannose C-1-00053



α-D-Pyranose-*form*

$C_6H_{11}ClO_5$ M 198.6

D-form [4990-81-2]
Syrup.

α-D-Pyranose-form

Me glycoside: [4990-80-1].
$C_7H_{13}ClO_5$ M 212.6 Cryst. (propanol). Mp 75°. $[\alpha]_D^{30}$ +60 (c, 1.0 in H_2O).

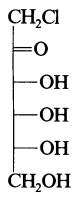
Me glycoside, 4-benzoyl, 2,3-di-Ac: [52290-42-3].
$C_{18}H_{21}ClO_8$ M 400.8 Cryst. Mp 120-121°. $[\alpha]_D^{25}$ +21 (c, 1.09 in $CHCl_3$).

Me glycoside, tribenzoyl:
$C_{28}H_{25}ClO_8$ M 524.9 Cryst. (MeOH). Mp 181-182°. $[\alpha]_D$ −115 (c, 0.4 in $CHCl_3$).

Me glycoside, 2,3-O-isopropylidene, 4-brosyl: [22932-32-7].
Cryst. (EtOH). Mp 121-122°. $[\alpha]_D^{24}$ −8.6 (c, 1.38 in MeOH).

Evans, M.E. *et al, J.O.C.*, 1968, **33**, 1074 (*α-Me pyr*)
Stevens, C.L. *et al, J.O.C.*, 1970, **35**, 592 (*brosyl, ms*)
Castro, B. *et al, Bull. Soc. Chim. Fr.*, 1973, 3034 (*α-Me pyr*)
Mathlouthi, M. *et al, Carbohydr. Res.*, 1986, **152**, 47 (D-form)

1-Chloro-1-deoxypsicose C-1-00054



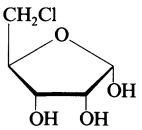
$C_6H_{11}ClO_5$ M 198.6

D-form

Tetra-Ac:
$C_{14}H_{19}ClO_9$ M 366.7 Cryst. Mp 89-91°. $[\alpha]_D$ −26 ($CHCl_3$).

Wolfrom, D. *et al, J.A.C.S.*, 1945, **67**, 1793 (*tetra-Ac*)

5-Chloro-5-deoxyribose C-1-00055



α-D-Furanose-*form*

$C_5H_9ClO_4$ M 168.5

α-D-Furanose-form

Me glycoside: Methyl 5-chloro-5-deoxy-α-D-ribofuranoside
$C_6H_{11}ClO_4$ M 182.6 Liq. $Bp_{0.3}$ 99-112°. $[\alpha]_D$ −19 (c, 1.0 in $CHCl_3$).

Me glycoside, 2,3-bis(chlorosulfate): [55053-19-5].
Cryst. Mp 115-116°. $[\alpha]_D$ +88 (c, 1.0 in $CHCl_3$).

β-D-Furanose-form

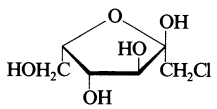
Me glycoside: Methyl 5-chloro-5-deoxy-β-D-ribofuranoside
$C_6H_{11}ClO_4$ M 182.6 Cryst. Mp 69.5-70.5°. $[\alpha]_D$ −65 (c, 1.0 in $CHCl_3$).

Me glycoside, 2,3-bis(chlorosulfate): [55053-21-9].
Cryst. Mp 78.5-79.5°. $[\alpha]_D$ +36 (c, 1.0 in $CHCl_3$).

Me glycoside, 2,3-O-isopropylidene: [38838-07-2].
$C_9H_{15}ClO_4$ M 222.6 Liq. $[\alpha]_D^{25}$ −93 (c, 2.04 in $CHCl_3$).

Hanessian, S. *et al, Carbohydr. Res.*, 1972, **24**, 45 (*β-Me gly deriv*)
Rabello, J.J. *et al, Carbohydr. Res.*, 1973, **30**, 381 (*β-Me gly deriv*)
Achmatowicz, B. *et al, Carbohydr. Res.*, 1974, **36**, C14 (*α-Me gly, β-Me gly*)

1-Chloro-1-deoxysorbose C-1-00056



α-L-Furanose-*form*

$C_6H_{11}ClO_5$ M 198.6

L-form [32785-89-0]
Syrup. Mp 95.5-97°. $[\alpha]_D$ −34.5 (c, 1.2 in H_2O).

α-L-Furanose-form

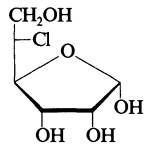
2,3-O-Isopropylidene: [32785-88-9].
$C_9H_{15}ClO_5$ M 238.6 Cryst. (EtOAc/petrol). Mp 71-72°. $[\alpha]_D$ +1.9 (c, 1.56 in H_2O).

2,3:4,6-Di-O-Isopropylidene: [32785-87-8].

$C_{12}H_{19}ClO_5$ M 278.7 Cryst. (petrol). Mp 56-58°. $Bp_{0.05}$ 83-86°. $[\alpha]_D$ −22.3 (c, 0.71 in $CHCl_3$).

Haylock, C.R. *et al*, *Carbohydr. Res.*, 1971, **16**, 375 (*synth*, L-form, α-L-fur derivs, pmr)
Beaupere, D. *et al*, *J. Carbohydr. Chem.*, 1989, **8**, 159 (*synth*, L-form)

5-Chloro-5-deoxytalose C-1-00057



β-L-Furanose-*form*

$C_6H_{11}ClO_5$ M 198.6

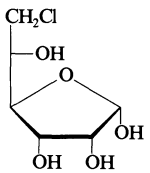
D-form [124729-12-0]
Syrup.

β-L-Furanose-form

1,2-O-Isopropylidene, 3-benzoyl, 6-Ac: [131289-38-8].
$C_{18}H_{21}ClO_7$ M 384.8 Syrup. $[\alpha]_D$ +66 (c, 0.8 in Me_2CO).

Pat. Coop. Treaty (*WIPO*), 89 07 602, (1989); *CA*, **112**, 99132k (D-form)
Lee, C.K., *Carbohydr. Res.*, 1990, **205**, 203 (β-L-fur deriv)

6-Chloro-6-deoxytalose C-1-00058



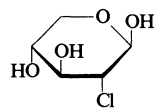
$C_6H_{11}ClO_5$ M 198.6

β-L-Furanose-form

1,2-O-Isopropylidene: [131289-41-3].
$C_9H_{15}ClO_5$ M 238.6 Cryst. Mp 146-148°. $[\alpha]_D$ +74 (c, 0.15 in EtOH).

Lee, C.K., *Carbohydr. Res.*, 1990, **205**, 203 (*isopropylidene, pmr*)

2-Chloro-2-deoxyxylose C-1-00059



β-D-Pyranose-*form*

$C_5H_9ClO_4$ M 168.5

D-Pyranose-form [29217-64-9]
Syrup. $[\alpha]_D$ +103.5 → + 163 (equilib.) (c, 1.0 in MeOH).

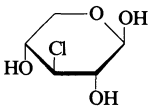
3,4-Di-Ac:
$C_9H_{13}ClO_6$ M 252.6 Mp 126°. $[\alpha]_D$ +49.9 ($CHCl_3$).

β-D-Pyranose-form

Me glycoside: [29217-63-8].
$C_6H_{11}ClO_4$ M 182.6 Cryst. ($CHCl_3$/petrol). Mp 136-137°. $[\alpha]_D^{21}$ −21 (c, 1.5 in MeOH).

Gakhokidze, A.M., *J. Gen. Chem. USSR* (*Engl. Transl.*), 1945, **15**, 530; *CA*, **40**, 4673 (*di-Ac*)
Jennings, H.J., *Can. J. Chem.*, 1970, **48**, 1834 (*β-Me gly*)

3-Chloro-3-deoxyxylose C-1-00060



β-D-Pyranose-*form*

$C_5H_9ClO_4$ M 168.5

β-D-Pyranose-form

Me glycoside: [18417-47-5].
$C_6H_{11}ClO_4$ M 182.6 Syrup. $Bp_{0.008}$ 135-140°. $[\alpha]_D$ −24.3 ($CHCl_3$).

Me glycoside, di-Ac: [18417-48-6].
$C_{10}H_{15}ClO_6$ M 266.6 Cryst. (EtOH aq.). Mp 116-117°. $[\alpha]_D$ −50 (c, 1.2 in $CHCl_3$).

α-D-Furanose-form

Me glycoside, 5-trityl: [40147-76-0].
$C_{25}H_{25}ClO_4$ M 424.9 Oil.

Me glycoside, 5-trityl, 2-(4-nitrobenzoyl): [40147-77-1].
Cryst. Mp 169-171°. $[\alpha]_D^{25}$ +90 (c, 1.0 in $CHCl_3$).

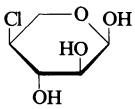
β-D-Furanose-form

Me glycoside, 5-trityl: [40147-71-5].
Glass.

Me glycoside, 5-trityl, 2-benzoyl: [40147-72-6].
$C_{32}H_{29}ClO_5$ M 529.0 Cryst. (C_6H_6/Et_2O/petrol). Mp 163-165°. $[\alpha]_D$ −10 (c, 1.0 in $CHCl_3$).

Allerton, R. *et al*, *J.C.S.*, 1951, 1480 (*Me pyr*)
Ali, S.S. *et al*, *Carbohydr. Res.*, 1967, **5**, 118 (*Me pyr*)
Jenkins, S.R. *et al*, *Carbohydr. Res.*, 1973, **26**, 71 (*Me fur, pmr*)

4-Chloro-4-deoxyxylose C-1-00061



α-L-Pyranose-*form*

$C_5H_9ClO_4$ M 168.5

α-L-Pyranose-form

Me glycoside, 2-mesyl: [18417-51-1].
$C_7H_{13}ClO_6S$ M 260.6 Cryst. (MeOH). Mp 119-120°. $[\alpha]_D$ −74 (c, 3.25 in $CHCl_3$).

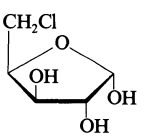
Me glycoside, 2-mesyl, 3-chlorosulfate: [18417-50-0].
$C_7H_{12}Cl_2O_8S_2$ M 359.2 Cryst. (MeOH). Mp 99-100°. $[\alpha]_D^{20}$ −38 (c, 5.4 in $CHCl_3$).

Me glycoside, 2,3-anhydro:
$C_6H_9ClO_3$ M 164.5 Syrup. Bp_{15} 40°. $[\alpha]_D$ −84 (c, 4.2 in $CHCl_3$).

β-L-Pyranose-form
Mp 128-131°. $[\alpha]_D$ +57 → 0 (MeOH).

Jones, J.K.N. *et al*, *Can. J. Chem.*, 1959, **37**, 1412; 1960, **38**, 1122 (β-L-pyr)
Ali, S.S. *et al*, *Carbohydr. Res.*, 1967, **5**, 118 (α-L-pyr derivs, ir)

5-Chloro-5-deoxyxylose C-1-00062



α-D-Furanose-*form*

$C_5H_9ClO_4$ M 168.5

α-D-Furanose-form

1,2-O-Isopropylidene: [105953-29-5].
$C_8H_{13}ClO_4$ M 208.6 Cryst. (diisopropyl ether/petrol). Mp 93-94° (91-92°).

1,2-O-Isopropylidene, 3-Ac: [61207-43-0].
$C_{10}H_{15}ClO_5$ M 250.6 Syrup.

1,2-O-Isopropylidene, 3-mesyl: [105953-28-4].
$C_9H_{15}ClO_6S$ M 286.7 Cryst. (diisopropyl ether). Mp 68-69°. $[\alpha]_D$ −77 (c, 1.0 in $CHCl_3$).

1,2-O-Isopropylidene, 3-chlorosulfate:
$C_8H_{12}Cl_2O_6S$ M 307.1 Cryst. Mp 96.5-97.5° (Et_2O/petrol). $[\alpha]_D$ −76 (c, 1.76 in $CHCl_3$).

Me glycoside: Methyl 5-chloro-5-deoxy-α-D-xylofuranoside
$C_6H_{11}ClO_4$ M 182.6 Cryst. Mp 73.5-74°. $[\alpha]_D$ +24 (c, 1.0 in MeOH).

Me glycoside, di-Ac: [56570-74-2].
$C_{10}H_{15}ClO_6$ M 266.6 Oil.

Me glycoside, dichlorosulfate:
$C_6H_9Cl_3O_8S_2$ M 379.6 Cryst. Mp 73.5-74.5°. $[\alpha]_D$ −15 (c, 1.0 in $CHCl_3$).

β-D-Furanose-form

1,2-Di-Ac, 3-chlorosulfate:
$C_9H_{12}Cl_2O_8S$ M 351.1 Cryst. (Et_2O/petrol). Mp 81.5-82°. $[\alpha]_D$ −105 (c, 1.2 in $CHCl_3$).

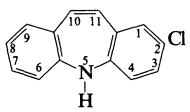
Me glycoside: Methyl 5-chloro-5-deoxy-β-D-xylofuranoside
$C_6H_{11}ClO_4$ M 182.6 Syrup. $[\alpha]_D$ −102 (c, 1.0 in MeOH).

Me glycoside, di-Ac: [56570-75-3].
$C_{10}H_{15}ClO_6$ M 266.6 Oil.

Achmatowicz, B. *et al*, *Carbohydr. Res.*, 1974, **36**, C14 (*α-Me fur, β-Me fur, dichlorosulfate*)
Hollenberg, D.H. *et al*, *Carbohydr. Res.*, 1975, **42**, 241 (*di-Ac, pmr*)
Hughes, N.A. *et al*, *J.C.S. Perkin 1*, 1986, 695 (*isopropylidene*)
Naidoo, N.T. *et al*, *S. Afr. J. Chem.*, 1986, **39**, 208; 1987, **40**, 100 (*3-chlorosulfate, ir, pmr, ms*)

2-Chloro-5*H*-dibenz[*b*,*f*] azepine C-1-00063

[22684-29-3]



$C_{14}H_{10}ClN$ M 227.6
Yellow plates (EtOH). Mp 168-170°.

Varma, R.S. *et al*, *J. Med. Chem.*, 1969, **12**, 913 (*synth*)
Molock, F.F. *et al*, *J. Het. Chem.*, 1983, **20**, 109 (*cmr*)
Tokmakov, G.P. *et al*, *Tetrahedron*, 1995, **51**, 2091 (*synth, uv, pmr*)

3-Chloro-5*H*-dibenz[*b*,*f*] azepine C-1-00064

[39607-90-4]

$C_{14}H_{10}ClN$ M 227.6
Orange-yellow plates (C_6H_6). Mp 213-214° (208-209°).

Craig, P.N. *et al*, *J.O.C.*, 1961, **26**, 135 (*synth, uv, ir*)
Kohegyi, I. *et al*, *J. Chem. Res., Synop.*, 1994, 270 (*synth, pmr, ms*)

10-Chloro-5*H*-dibenz[*b*,*f*]azepine C-1-00065

[59691-00-8]

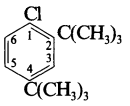
$C_{14}H_{10}ClN$ M 227.6

Ger. Pat., 2 542 335, (1976); *CA*, **85**, 32888s (*synth*)

1-Chloro-2,4-di-*tert*-butylbenzene C-1-00066

1-Chloro-2,4-bis(1,1-dimethylethyl)benzene

[80438-65-9]



$C_{14}H_{21}Cl$ M 224.7
Oil. $Bp_{0.5}$ 80°.

de Konig, A.J., *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1981, **100**, 421; 1982, **101**, 385 (*synth, pmr*)
Dehmlow, E.V. *et al*, *Tetrahedron*, 1995, **51**, 3755 (*synth*)

1-Chloro-3,5-di-*tert*-butylbenzene C-1-00067

1-Chloro-3,5-bis(1,1-dimethylethyl)benzene

[80438-67-1]

$C_{14}H_{21}Cl$ M 224.7
Cryst. Mp 54-55°.

de Konig, A.J., *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1981, **100**, 421; 1982, **101**, 385 (*synth, pmr*)

2-Chloro-1,3-di-*tert*-butylbenzene C-1-00068

2-Chloro-1,3-bis(1,1-dimethylethyl)benzene

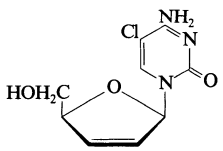
[84363-20-2]

$C_{14}H_{21}Cl$ M 224.7
Oil.

de Konig, A.J., *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1981, **100**, 421; 1982, **101**, 385 (*synth, pmr*)

5-Chloro-2′,3′-didehydro-2′,3′-dideoxycytidine, 9CI C-1-00069

[124743-30-2]

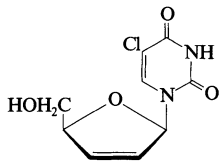


$C_9H_{10}ClN_3O_3$ M 243.6
Cryst. (MeOH/Et_2O). Mp 144-145°.

Van Aerschot, A. *et al*, *J. Med. Chem.*, 1990, **33**, 1833 (*synth, uv, pmr, cmr, ms*)

5-Chloro-2′,3′-didehydro-2′,3′-dideoxyuridine, 9CI C-1-00070

[120815-05-6]

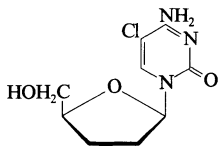


$C_9H_9ClN_2O_4$ M 244.6
Cryst. (MeOH/Et_2O). Mp 140-142° dec.

Van Aerschot, A. *et al*, *J. Med. Chem.*, 1990, **33**, 1833 (*synth, uv, ms, pmr, cmr*)

5-Chloro-2′,3′-dideoxycytidine, 9CI C-1-00071

[124743-31-3]

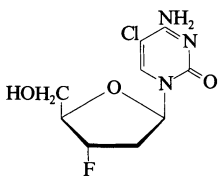


$C_9H_{12}ClN_3O_3$ M 245.6
Cryst. Mp 172°.

Van Aerschot, A. *et al*, *J. Med. Chem.*, 1990, **33**, 1833 (*synth, uv, pmr, ms, cmr*)

5-Chloro-2′,3′-dideoxy-3′-fluorocytidine, 9CI C-1-00072

[127492-32-4]

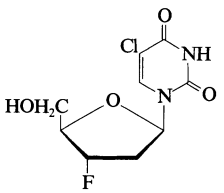


$C_9H_{11}ClFN_3O_3$ M 263.6
Cryst. (MeOH/Me_2CO). Mp 184-185°.

Van Aerschot, A. *et al*, *J. Med. Chem.*, 1990, **33**, 1833 (*synth, uv, pmr, cmr, ms*)

5-Chloro-2′,3′-dideoxy-3′-fluorouridine, 9CI C-1-00073

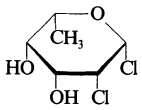
[119644-22-3]



$C_9H_{10}ClFN_2O_4$ M 264.6
Selective inhibitor of HIV-1 and HIV-2 replication. Cryst. (Me_2CO/hexane). Mp 181° dec. (exp.).

Van Aerschot, A. *et al*, *J. Med. Chem.*, 1989, **32**, 1743; 1990, **33**, 1833 (*synth, uv, ms, pmr, cmr, cryst struct*)

2-Chloro-2,6-dideoxytalopyranosyl chloride C-1-00074



$C_6H_{10}Cl_2O_3$ M 201.0

β-L-form

Di-Ac: [103321-23-9].
$C_{10}H_{14}Cl_2O_5$ M 285.1 Syrup. $[\alpha]_D^{23}$ +4 (c, 0.4 in CH_2Cl_2).

Horton, D. *et al*, *J.O.C.*, 1986, **51**, 3479 (*di-Ac, ir, ms, pmr, cmr*)

2-Chloro-3,4-difluorobenzoic acid C-1-00075

$C_7H_3ClF_2O_2$ M 192.5
Cryst. solid (heptane/Et_2O). Mp 159-160°.

Bennetau, B. *et al*, *J.C.S. Perkin 1*, 1995, 1265 (*synth, pmr, cmr*)

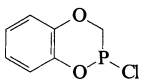
3-Chloro-2,4-difluorobenzoic acid C-1-00076

$C_7H_3ClF_2O_2$ M 192.5
Cryst. solid (heptane/Et_2O). Mp 169-171°.

Bennetau, B. *et al*, *J.C.S. Perkin 1*, 1995, 1265 (*synth, pmr*)

2-Chloro-2,3-dihydro-1,4,2-benzodioxaphosphorin, 9CI C-1-00077

[124167-64-2]



$C_7H_6ClO_2P$ M 188.5
Liq. d_4^{20} 1.39. Bp_4 105-106°. n_D^{20} 1.5990.

2-Oxide: [110606-92-3].
$C_7H_6ClO_3P$ M 204.5 Liq. d_4^{20} 1.48. $Bp_{1.5}$ 123-124°. n_D^{20} 1.5568.

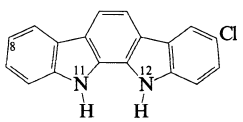
2-Sulfide: [124167-63-1].
$C_7H_6ClO_2PS$ M 220.6 Liq. d_4^{20} 1.61. Bp_1 102-103°. n_D^{20} 1.4316.

Tsvetkov, E.N. *et al*, *Zh. Obshch. Khim.*, 1986, **56**, 2542; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1986, **56**, 2249 (*oxide*)
Degtyarev, A.N. *et al*, *Zh. Obshch. Khim.*, 1988, **58**, 2226; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1988, **58**, 1982 (*synth, pmr, P-31 nmr*)

3-Chloro-11,12-dihydroindolo[2,3-*a*]carbazole, 9CI C-1-00078

Tjipanazole I

[139083-26-4]



$C_{18}H_{11}ClN_2$ M 290.7
Minor alkaloid from the blue-green alga *Tolypothrix tjipanasensis.*

N^{11}-(*6-Deoxy-β-D-gulopyranosyl*): ***Tjipanazole C1***
$C_{24}H_{21}ClN_2O_4$ M 436.8 Minor alkaloid from blue-green alga *Tolypothrix tjipanasensis.* $[\alpha]_D$ +18.1 (c, 1.1 in $CHCl_3$). Opt. rotn. refers to a mixt. with other Tjipanazole C components.

N^{11}-*α-L-Rhamnopyrannosyl:* ***Tjipanazole C3***
$C_{24}H_{21}ClN_2O_4$ M 436.8 Minor constit. of *T. tjipanasensis.*

N^{11}-*β-D-Xylopyranosyl:* ***Tjipanazole F1***
$C_{23}H_{19}ClN_2O_4$ M 422.8 Minor alkaloid from *T. tjipanasensis.* $[\alpha]_D$ +14.9 (c, 1.0 in $CHCl_3$/MeOH 1:1). Opt. rotn. refers to a mixt. with F2.

N^{12}-*β-D-Xylopyranosyl:* ***Tjipanazole F2***
$C_{23}H_{19}ClN_2O_4$ M 422.8 Minor alkaloid from *T. tjpanasensis.*

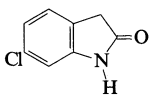
N^{12}-(*6-Deoxy-β-D-gulopyranosyl*): ***Tjipanazole C2***
$C_{24}H_{21}ClN_2O_4$ M 436.8 Minor constit. of *T. tjipanasensis.*

N^{12}-*α-L-Rhamnopyranosyl:* ***Tjipanazole C4***
$C_{24}H_{21}ClN_2O_4$ M 436.8 Minor constit. of *T. tjipanasensis.*

Bonjouklian, R. *et al*, *Tetrahedron*, 1991, **47**, 7739 (*isol, uv, pmr, struct*)

6-Chloro-1,3-dihydro-2*H*-indol-2-one, 9CI C-1-00079

6-Chlorooxindole. 6-Chloro-2-indolinone
[56341-37-8]

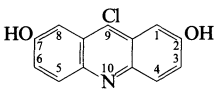


C_8H_6ClNO M 167.5
Cryst. Mp 196-198° (189-192°).

Quallich, G.J. *et al*, *Synthesis*, 1993, 51 (*synth, pmr*)

9-Chloro-2,7-dihydroxyacridine C-1-00080

9-Chloro-2,7-acridinediol, 9CI
[156644-26-7]



$C_{13}H_8ClNO_2$ M 245.6
Solid. Mp >300°.

Vichet, A. *et al*, *J.O.C.*, 1994, **59**, 5156 (*synth, pmr*)

4-Chloro-3,5-dihydroxybenzaldehyde C-1-00081

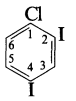
$C_7H_5ClO_3$ M 172.5

Di-Me ether: [56518-48-0]. *4-Chloro-3,5-dimethoxybenzaldehyde*
$C_9H_9ClO_3$ M 200.6 Isol. from the mycelium of *Hericium erinaceum.* Exhibits antibacterial activity. Cryst. Mp 165-167° (118-120°).

Kompis, I. *et al*, *Helv. Chim. Acta*, 1977, **60**, 3025 (*synth*)
Okamoto, K. *et al*, *Phytochemistry*, 1993, **34**, 1445 (*isol*)

1-Chloro-2,4-diiodobenzene C-1-00082

[31928-48-0]



$C_6H_3ClI_2$ M 364.3
Bp_2 129°.

Bunnett, J.F. *et al*, *J.A.C.S.*, 1971, **93**, 1183 (*synth*)

1-Chloro-3,5-diiodobenzene C-1-00083

$C_6H_3ClI_2$ M 364.3
Needles (EtOH). Mp 101°.

Dains, F.B. *et al*, *J.A.C.S.*, 1930, **52**, 1572 (*synth*)

2-Chloro-1,3-diiodobenzene C-1-00084

$C_6H_3ClI_2$ M 364.3
Cryst. (EtOH). Mp 82°.

Körner, G. *et al*, *Atti Accad. Naz. Lincei, Cl. Sci. Fis., Mat. Nat., Rend.*, 1913, **22**, 832 (*synth*)

2-Chloro-1,4-diiodobenzene C-1-00085

[79887-23-3]

$C_6H_3ClI_2$ M 364.3
Cryst. (EtOH). Mp 51°.

Körner, G. *et al*, *Atti Accad. Naz. Lincei, Cl. Sci. Fis., Mat. Nat., Rend.*, 1913, **22**, 832 (*synth*)
Adomenas, P. *et al*, *CA*, 1981, **95**, 219871e.

4-Chloro-1,2-diiodobenzene, 9CI C-1-00086

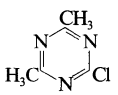
[1608-45-3]

$C_6H_3ClI_2$ M 364.3
Slightly yellow cryst. (hexanes). Mp 34-35°, Mp 39-40.5°.

Bunnett, J.F. *et al*, *J.A.C.S.*, 1930, **52**, 1572 (*synth*)
Perry, R.J. *et al*, *J.O.C.*, 1991, **56**, 6573 (*synth, pmr, ir*)

2-Chloro-4,6-dimethyl-1,3,5-triazine, 9CI C-1-00087

[30894-84-9]

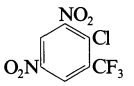


$C_5H_6ClN_3$ M 143.5
Cryst. (petrol). Mp 64°.

Schroeder, H. *et al*, *J.A.C.S.*, 1956, **78**, 2447 (*synth*)

2-Chloro-1,5-dinitro-3-(trifluoromethyl)benzene, 9CI C-1-00088

2-Chloro-α,α,α-trifluoro-3,5-nitrotoluene, 8CI. 2-Chloro-3,5-dinitrobenzotrifluoride
[392-95-0]



$C_7H_2ClF_3N_2O_4$ M 270.5
Cryst. (EtOH). Mp 62-64° (58°).

[82668-92-6]

U.S. Pat., 2 257 093, (1940); *CA*, **36**, 664a (*synth*)
Yagupol'skii, L.M. *et al*, *CA*, 1955, **49**, 8866i (*synth*)

2-Chlorodiphenylmethanol C-1-00089

2-Chloro-α-phenylbenzenemethanol, 9CI. 2-Chlorobenzhydrol, 8CI
[6954-45-6]

$C_{13}H_{11}ClO$ M 218.6

(+)-***form***
$[\alpha]_D$ +21.3 (c, 0.5 in Me_2CO) (ee 100%).

(−)-***form***
Mp 65-66°. $[\alpha]_D^{20}$ −19.9 (c, 0.52 in Me_2CO) (ee >95%).

(±)-***form*** [134236-27-4]
Needles (petrol). Mp 65°.

[16071-25-3, 16071-26-4]

Koopal, S.A., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1915, **34**, 8, 158 (*synth*)
Balfe, M.P. *et al*, *J.C.S.*, 1946, 797 (*resoln*)
Bachmann, W.E. *et al*, *J.O.C.*, 1948, **13**, 916 (*synth*)
Wang, J.-T. *et al*, *Synthesis*, 1989, 291 (*synth, ir, pmr*)
Brown, E. *et al*, *Tetrahedron: Asymmetry*, 1991, **2**, 339 (*synth*)

3-Chlorodiphenylmethanol C-1-00090

3-Chloro-α-phenylbenzenemethanol, 9CI. 3-Chlorobenzhydrol, 8CI
[63012-03-3]

$C_{13}H_{11}ClO$ M 218.6

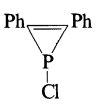
(+)-***form*** [123436-12-4]
Mp 40-41°. $[\alpha]_D^{20}$ +30.3 (c, 1.12 in Me_2CO) (>95% ee).

(±)-***form*** [134172-63-7]
Cryst. (petrol). Mp 40°.

Koopal, S.A., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1915, **34**, 8, 158 (*synth*)
Bachmann, W.E. *et al*, *J.O.C.*, 1948, **13**, 916 (*synth*)
Wang, J.-T. *et al*, *Synthesis*, 1989, 291 (*synth, ir, pmr*)

1-Chloro-2,3-diphenyl-1*H*-phosphirene C-1-00091

[123120-23-0]

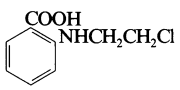


$C_{14}H_{10}ClP$ M 244.6
Cryst. Mp 91°. $Bp_{0.002}$ 200° (oven).

Deschamps, B. *et al*, *Nouv. J. Chim.*, 1988, **12**, 755 (*formn*)
Schmurr, W. *et al*, *Tet. Lett.*, 1989, **30**, 3951 (*synth*, *cmr*, *P-31 nmr*)

2-[(2-Chloroethyl)amino]benzoic acid C-1-00092

N-(*2-Chloroethyl*)*anthranilic acid*



$C_9H_{10}ClNO_2$ M 199.6
Platelets (petrol). Mp 115-116°.

Me ester:
$C_{10}H_{12}ClNO_2$ M 213.6 Platelets (pentane). Mp 35°.

Amide: [88267-60-1].
$C_9H_{11}ClN_2O$ M 198.6 Needles (2-propanol/diisopropyl ether). Mp 126-127°.

Everett, J.L. *et al*, *J.C.S.*, 1953, 2386 (*synth*, *Me ester*)
Yamada, Y. *et al*, *Chem. Pharm. Bull.*, 1983, **31**, 2234 (*amide*)

4-[(2-Chloroethyl)amino]benzoic acid C-1-00093

[2045-23-0]

$C_9H_{10}ClNO_2$ M 199.6
Cryst. Mp 175° dec.

Hydrochloride: Needles (Me_2CO). Mp 215°.
Et ester:
$C_{11}H_{14}ClNO_2$ M 227.6 Cryst. Mp 69°.

Bardos, T.J. *et al*, *J. Med. Chem.*, 1965, **8**, 167 (*synth*)
Lee, M. *et al*, *Synth. Commun.*, 1994, **24**, 3129 (*synth*, *pmr*, *cmr*, *ir*)

(Chloroethynyl)phosphonic acid C-1-00094

Chloroacetylenephosphonic acid

$ClC{\equiv}CP(O)(OH)_2$

$C_2H_2ClO_3P$ M 140.4

Di-Me ester: Dimethyl chloroethynylphosphonate
$C_4H_6ClO_3P$ M 168.5 Liq. Bp_2 55°. n_D^{20} 1.4550.

Di-Et ester: Diethyl chloroethynylphosphonate
$C_6H_{10}ClO_3P$ M 196.5 Liq. d_4^{20} 1.15. $Bp_{2.5}$ 88.5-89.5°. n_D^{20} 1.4473.

Dipropyl ester: [72571-70-1]. *Dipropyl chloroethynylphosphonate*
$C_8H_{14}ClO_3P$ M 224.6 Liq. d_4^{20} 1.10. Bp_1 98-99°. n_D^{20} 1.4566.

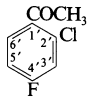
Diisopropyl ester: [41459-62-5]. *Bis(1-methylethyl) chloroethynylphosphonate*
Sl. yellow liq. n_D^{20} 1.417.

Ionin, B.I. *et al*, *Zh. Obshch. Khim.*, 1965, **35**, 1917; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1965, **35**, 1910 (*synth*)
Seyferth, D. *et al*, *J.O.C.*, 1969, **34**, 1483 (*synth*, *ir*, *pmr*)
Maier, L., *Phosphorus Relat. Group V Elem.*, 1973, **2**, 229 (*synth*, *pmr*, *P-31 nmr*)
Kruglov, S.V. *et al*, *Zh. Obshch. Khim.*, 1973, **43**, 1480; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1973, **43**, 1470 (*synth*, *pmr*)
Garabina, V.A. *et al*, *Zh. Obshch. Khim.*, 1979, **49**, 1964; 1985, **55**, 1994; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1979, **49**, 1728; 1985, **55**, 1771 (*ir*, *cmr*, *ms*, *P-31 nmr*, *props*)

2′-Chloro-4′-fluoroacetophenone, 8CI C-1-00095

1-(2-Chloro-4-fluorophenyl)ethanone, *9CI. 1-Acetyl-2-chloro-4-fluorobenzene*

[700-35-6]



C_8H_6ClFO M 172.5
Bp_{19} 110°. n_D^{24} 1.5310.

Oxime:
C_8H_7ClFNO M 187.6 Needles. Mp 131°.

2,4-Dinitrophenylhydrazone: Red needles (AcOH). Mp 167°.
Semicarbazone: Prisms (EtOH). Mp 193°.

Diep, B.K. *et al*, *J.C.S.*, 1963, 2784 (*synth*, *ir*)

3′-Chloro-4′-fluoroacetophenone C-1-00096

1-(3-Chloro-4-fluorophenyl)ethanone. 4-Acetyl-2-chloro-1-fluorobenzene

[2923-66-2]

C_8H_6ClFO M 172.5
Flat prisms (pentane). Mp 41-42°. Bp 226°, Bp_{15} 126-128°.

Oxime:
C_8H_7ClFNO M 187.6 Cryst. (EtOH). Mp 97°.

Phenylhydrazone: Mp 116-119°.
2,4-Dinitrophenylhydrazone: Red prisms (AcOH). Mp 238°.
Semicarbazone: Cryst. (EtOH). Mp 212-213.5°.

Baltzly, R. *et al*, *J.O.C.*, 1961, **26**, 2353 (*synth*)
Diep, B.K. *et al*, *J.C.S.*, 1963, 2784 (*synth*, *ir*)

2-Chloro-3-fluorobenzoic acid C-1-00097

$C_7H_4ClFO_2$ M 174.5
Cryst. solid (heptane/Et_2O). Mp 169-171°.

Bennetau, B. *et al*, *J.C.S. Perkin 1*, 1995, 1265 (*synth*, *pmr*, *F-19 nmr*, *cmr*)

2-Chloro-3-furancarboxaldehyde C-1-00098

2-Chloro-3-furaldehyde, *8CI. 2-Chloro-3-formylfuran*

[31491-42-6]

$C_5H_3ClO_2$ M 130.5
Liq. Bp_{20} 64°.

Roques, B. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 242 (*synth*, *pmr*)

4-Chloro-2-furancarboxaldehyde, 9CI C-1-00099

4-Chlorofurfural. 4-Chloro-2-formylfuran

[57500-47-7]

$C_5H_3ClO_2$ M 130.5
Cryst. (petrol). Mp 27-29°.

Oxime: [57635-14-0].
$C_5H_4ClNO_2$ M 145.5 Cryst. (EtOH). Mp 135°.

2,4-Dinitrophenylhydrazone: [57635-17-3]. Red cryst. (EtOH). Mp 229°.
Semicarbazone: [57635-15-1]. Mp 222°.

Belen'kii, L.I. *et al*, *Khim. Geterotsikl. Soedin.*, 1975, 1464; *Chem. Heterocycl. Compd.* (*Engl. Transl.*), 1975, 1249 (*synth*, *pmr*)
Nazarova, Z.N. *et al*, *Zh. Org. Khim.*, 1975, **11**, 1955; *J. Org. Chem. USSR* (*Engl. Transl.*), 1975, **11**, 1974 (*synth*, *derivs*, *pmr*, *uv*, *ir*)

5-Chloro-2-furancarboxaldehyde, 9CI C-1-00100

5-Chlorofurfural. 2-Chloro-5-formylfuran

[21508-19-0]

$C_5H_3ClO_2$ M 130.5
Cryst. (hexane). Mp 35-36° (30.5-31°). Bp_{755} 180°.

Oxime:
$C_5H_4ClNO_2$ M 145.5 Cryst. (EtOH aq.). Mp 84°.

Semicarbazone: [42899-89-8]. Cryst. (2-propanol). Mp 199-201°.

Gilman, H. *et al*, *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1931, **50**, 833 (*synth*, *oxime*)
Chute, W.J. *et al*, *J.O.C.*, 1945, **10**, 541 (*synth*)
Nazarova, Z.N. *et al*, *Zh. Obshch. Khim.*, 1962, **32**, 723; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1962, **32**, 721 (*synth*, *oxime*)
Snyder, H.R. *et al*, *J. Het. Chem.*, 1973, **10**, 385 (*synth*, *pmr*, *ir*)
D'Auria, M. *et al*, *Synthesis*, 1995, 248 (*synth*)

2-Chloro-1,1,1,3,4,4,4-heptafluoro-2-butene C-1-00101

[434-41-3]

$F_3CCCl{=}CFCF_3$

C_4ClF_7 M 216.4
d 1.55. Bp 32°. n_D^{20} 1.2946.

[5953-44-6, 5954-49-4]

Henne, A.L. *et al*, *J.A.C.S.*, 1948, **70**, 130 (*synth*)
U.S. Pat., 2 436 357, (1948); *CA*, **42**, 5465e.
Saloutina, L.V. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1968, **6**, 1360; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1988, **6**, 1196 (*synth*, *F-19 nmr*, *ir*)

4-Chloro-1,1,2,3,3,4,4-heptafluoro-1-butene C-1-00102

[378-81-4]

$F_2C{=}CFCF_2CF_2Cl$

C_4ClF_7 M 216.4
Bp 29-35°. n_D^{20} 1.299.

U.S. Pat., 2 886 607, (1959); *CA*, **53**, 17903b.

1-Chloro-2-hexanone C-1-00103

[20261-68-1]

$H_3C(CH_2)_3COCH_2Cl$

$C_6H_{11}ClO$ M 134.6
Liq. Bp_{12} 68-70°. n_D^{24} 1.4360.

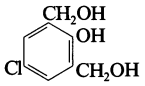
Bunnett, J.F. *et al*, *J.A.C.S.*, 1945, **67**, 1944 (*synth*)

Archer, D. *et al*, *J.A.C.S.*, 1956, **78**, 6182 (*synth*)
Cadman, M.L.F. *et al*, *J.C.S. Perkin 1*, 1995, 1397 (*synth, ir, pmr*)

5-Chloro-2-hydroxy-1,3-benzenedimethanol, 9CI C-1-00104

*5-Chloro-2-hydroxy-*m*-xylene-α,α′-diol, 8CI. 4-Chloro-2,6-bis(hydroxymethyl)phenol. Ferriphene*

[17026-49-2]



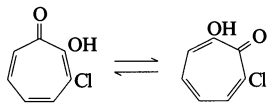
$C_8H_9ClO_3$ M 188.6
Reagent for detn. of iron. Cryst. (H_2O). Mp 164°.

Foster, H.M. *et al*, *J.O.C.*, 1961, **26**, 2539 (*synth*)
Rodia, J.S., *J.O.C.*, 1961, **26**, 2966 (*synth*)
Chen, Z. *et al*, *Huaxue Xuebao*, 1982, **40**, 135; *CA*, **97**, 16255a (*synth, use*)

3-Chloro-2-hydroxy-2,4,6-cycloheptatrien-1-one C-1-00105

2-Chloro-7-hydroxy-2,4,6-cycloheptatrien-1-one. 3-Chlorotropolone

[824-29-3]



$C_7H_5ClO_2$ M 156.5
Needles or prisms (EtOH). Mp 103-104° (100-102°), Mp 112-113°.

Nozoe, T. *et al*, *CA*, 1955, **49**, 8240f (*synth*)
Takase, K., *Bull. Chem. Soc. Jpn.*, 1964, **37**, 1288 (*synth, uv*)
Tsuji, T. *et al*, *Acta Cryst. C*, 1991, **47**, 2428 (*cryst struct*)

4-Chloro-2-hydroxy-2,4,6-cycloheptatrien-1-one C-1-00106

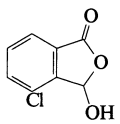
6-Chloro-2-hydroxy-2,4,6-cycloheptatrien-1-one. 4-Chlorotropolone

[698-48-6]

$C_7H_5ClO_2$ M 156.5
Needles (EtOH). Mp 79-80°.

Sato, T., *Nippon Kagaku Kaishi*, 1959, **80**, 1171; *CA*, **55**, 4389d (*synth*)
Takase, K., *Bull. Chem. Soc. Jpn.*, 1964, **37**, 1298 (*synth*)

4-Chloro-3-hydroxy-3*H*-isobenzofuran-1-one C-1-00107



$C_8H_5ClO_3$ M 184.5

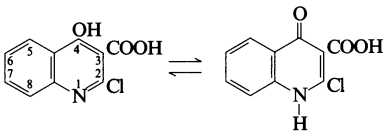
(±)-form
Cryst. solid (heptane/Et_2O). Mp 124-126°.

Bennetau, B. *et al*, *J.C.S. Perkin 1*, 1995, 1265 (*synth, pmr, cmr*)

2-Chloro-4-hydroxy-3-quinolinecarboxylic acid C-1-00108

2-Chloro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid

[99429-63-7]



$C_{10}H_6ClNO_3$ M 223.6
CAS no. refers to the oxo-tautomer. Mp 196°.

Brown, R.F.C. *et al*, *Aust. J. Chem.*, 1954, **7**, 348.

6-Chloro-4-hydroxy-3-quinolinecarboxylic acid C-1-00109

6-Chloro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid

[35973-14-9]

$C_{10}H_6ClNO_3$ M 223.6
Cryst. ($PhNO_2$). Mp 277° (261° dec.).

Et ester: [70271-77-1].
$C_{12}H_{10}ClNO_3$ M 251.6 Cryst. ($PhNO_2$). Mp 293°.

[53977-19-8]

Riegel, B. *et al*, *J.A.C.S.*, 1946, **68**, 1264.
Duffin, G.F. *et al*, *J.C.S.*, 1948, 893.
Roberts, R., *J.O.C.*, 1951, **14**, 285.

7-Chloro-4-hydroxy-3-quinolinecarboxylic acid C-1-00110

7-Chloro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid

[57278-46-3]

$C_{10}H_6ClNO_3$ M 223.6
CAS no. refers to the oxo-tautomer. Needles (EtOH). Mp 274° dec.

Et ester: [16600-22-9].
$C_{12}H_{10}ClNO_3$ M 251.6 Cryst. (Py). Mp 297°.

[86-47-5]

Price, C.C. *et al*, *J.A.C.S.*, 1946, **68**, 1204.
Duffin, G.F. *et al*, *J.C.S.*, 1948, 893.
Roberts, R., *J.O.C.*, 1951, **14**, 285.

8-Chloro-4-hydroxy-3-quinolinecarboxylic acid C-1-00111

8-Chloro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid

[35966-16-6]

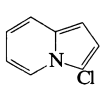
$C_{10}H_6ClNO_3$ M 223.6
Mp 258° dec.

[35975-71-4]

Roberts, R., *J.O.C.*, 1951, **14**, 285.

3-Chloroindolizine, 9CI C-1-00112

[63359-55-7]



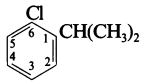
C_8H_6ClN M 151.5
Liq. Unstable; turns black within 1h.

Berg-Nielsen, K., *Acta Chem. Scand., Ser. B*, 1977, **31**, 224 (*synth, uv, pmr, ms*)
Bonneau, R. *et al*, *Chem. Comm.*, 1994, 509 (*synth, pmr*)

1-Chloro-2-isopropylbenzene C-1-00113

1-Chloro-2-(1-methylethyl)benzene, 9CI. 2-Chlorocumene, 8CI

[2077-13-6]



$C_9H_{11}Cl$ M 154.6
Liq. Bp_{746} 193°.

Kiersznicki, T. *et al*, *CA*, 1968, **68**, 12579n (*synth*)
Smith, K. *et al*, *Synthesis*, 1985, 1155, 1157 (*synth*)
Adv. Chem. Ser., 1955, **15**, 148 (***props***)

1-Chloro-3-isopropylbenzene C-1-00114

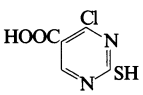
1-Chloro-3-(1-methylethyl)benzene, 9CI. m-*Chlorocumene, 8CI*

[7073-93-0]

$C_9H_{11}Cl$ M 154.6
Liq. Bp_{746} 193-194°.

Kiersnicki, T. *et al*, *CA*, 1968, **68**, 12579n (*synth*)
Reetz, M.T. *et al*, *Chem. Ber.*, 1987, **120**, 123 (*synth*)
Katayoma, T. *et al*, *Chem. Lett.*, 1991, 2073 (*synth*)

4-Chloro-2-mercapto-5-pyrimidinecarboxylic acid, 9CI C-1-00115



$C_5H_3ClN_2O_2S$ M 190.6
Parent compd. unknown (1994). Two *NH* tautomers also possible.

S-*Me, Me ester:* [38275-39-7].
$C_7H_7ClN_2O_2S$ M 218.6 Cryst. (MeOH aq.). Mp 76-78°.

S-*Me, Et ester:* [5909-24-0].
$C_8H_9ClN_2O_2S$ M 232.6 Cryst. (petrol). Mp 60-63°.
▶ Mild vesicant.

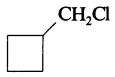
S-*Me, nitrile:* [33089-15-5]. *4-Chloro-5-cyano-2-(methylthio)pyrimidine*
$C_6H_4ClN_3S$ M 185.6 Cryst. (pentane). Mp 61-63°.

S-*Me, anhydride:* [62094-69-3].
$C_{12}H_8Cl_2N_4O_3S_2$ M 391.2 Cryst. (hexane). Mp 117-118°.

Todd, C.W. *et al*, *J.A.C.S.*, 1943, **65**, 352 (*synth*)
Shadbolt, R.S. *et al*, *J.C.S.(C)*, 1967, 1172 (*synth*)
Santilli, A.A. *et al*, *J. Het. Chem.*, 1971, **8**, 445 (*nitrile*)
Budesinsky, Z. *et al*, *Coll. Czech. Chem. Comm.*, 1972, **37**, 1721 (*synth, Me ester*)
Kimura, Y. *et al*, *Chem. Pharm. Bull.*, 1976, **24**, 2637 (*anhydride*)

(Chloromethyl)cyclobutane C-1-00116

Cyclobutylmethyl chloride

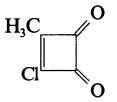


C_5H_9Cl M 104.5
Bp 109-111°. n_D^{21} 1.448.

Richey, H.G. *et al*, *J.O.C.*, 1964, **29**, 421.
Beckwith, A.L.J. *et al*, *J.C.S. Perkin 2*, 1980, 1083.

3-Chloro-4-methyl-3-cyclobutene-1,2-dione, 9CI C-1-00117

[75966-10-8]



$C_5H_3ClO_2$ M 130.5
Yellow oil or cryst. (Et_2O/hexane). Mp 31-32°. Bp_{18} 80-88° ($Bp_{0.5}$ 75-80°).

Bellus, D. *et al*, *Helv. Chim. Acta*, 1980, **65**, 1130 (*synth*, *uv*, *ir*, *pmr*)
Liebeskind, L.S. *et al*, *J.A.C.S.*, 1993, **115**, 9048 (*synth*, *ir*, *pmr*)

(Chloromethylene) dimethylammonium(1+) C-1-00118

$ClCH{=}NMe_2^{\oplus}$

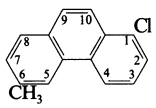
$C_3H_7ClN^{\oplus}$ M 92.5 (ion)

Chloride: Dimethylformamide chloride
$C_3H_7Cl_2N$ M 128.0 Obt. from Dimethylformamide, D-0-09491 + phosgene, $SOCl_2$ or PCl_5. Cryst. Mp 140-145°. V. hygroscopic, hydrol. by H_2O. Stable under N_2 at least 1 month.

Bosshard, H.H. *et al*, *Helv. Chim. Acta*, 1959, **42**, 1653.

1-Chloro-6-methylphenanthrene, 9CI C-1-00119

[84194-40-1]



$C_{15}H_{11}Cl$ M 226.7
Cryst. (petrol). Mp 99.6-100.2°.

Mallory, F.B. *et al*, *J.O.C.*, 1983, **48**, 526 (*synth*)

9-Chloro-10-methylphenanthrene, 9CI C-1-00120

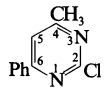
[52979-77-8]

$C_{15}H_{11}Cl$ M 226.7
Pale beige needles (EtOH). Mp 120-121°.

Washburn, L.C. *et al*, *J. Med. Chem.*, 1974, **17**, 676 (*synth*)
Pearson, D.E. *et al*, *Synthesis*, 1976, 621 (*synth*)

2-Chloro-4-methyl-6-phenylpyrimidine, 9CI C-1-00121

[32785-40-3]



$C_{11}H_9ClN_2$ M 204.6
Cryst. Mp 53° (50-51°).

Merkatz, A.V., *Ber.*, 1919, **52**, 869 (*synth*)
Elmoghayar, M.R.H. *et al*, *Acta Chem. Scand., Ser. B*, 1983, **37**, 109 (*synth*, *pmr*, *ms*)

4-Chloro-2-methyl-6-phenylpyrimidine, 9CI C-1-00122

[2915-15-3]

$C_{11}H_9ClN_2$ M 204.6
Cryst. (petrol). Mp 59°.

Streef, J.W. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1969, **88**, 1391 (*synth*)
Marsura, A. *et al*, *Synthesis*, 1993, 478 (*synth*, *pmr*, *ms*)

4-Chloro-6-methyl-2-phenylpyrimidine, 9CI C-1-00123

6-Chloro-4-methyl-2-phenylpyrimidine

[29509-92-0]

$C_{11}H_9ClN_2$ M 204.6
Cryst. (hexane or petrol). Mp 73-74°.

Crenshaw, R.R. *et al*, *J. Het. Chem.*, 1970, **7**, 871 (*synth*)
Kato, T. *et al*, *Org. Mass Spectrom.*, 1974, **9**, 981 (*ms*)
Honma, Y. *et al*, *Chem. Pharm. Bull.*, 1982, **30**, 4314 (*synth*, *ms*)

P-(Chloromethyl)phosphonous diamide, 9CI C-1-00124

$ClCH_2P(NH_2)_2$

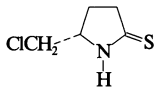
CH_6ClN_2P M 112.4

N,N,N′,N′-*Tetra-Et:* [100548-25-2]. P-(*Chloromethyl*)-N,N,N′,N′-*tetraethylphosphonous diamide.* (*Chloromethyl*)*phosphonous bis*(*diethylamide*)
$C_9H_{22}ClN_2P$ M 224.7 Oil.

N,N,N′,N′-*Tetraisopropyl:* [124862-12-0]. P-(*Chloromethyl*)-N,N,N′,N′-*tetraisopropylphosphonous diamide.* (*Chloromethyl*)*phosphonous bis*(*diisopropylamide*)
$C_{13}H_{30}ClN_2P$ M 280.8 Cryst. Mp 61° (31°).

Prishchenko, A.A. *et al*, *Zh. Obshch. Khim.*, 1985, **55**, 1194; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1985, **55**, 1065 (*tetraethyl*, *synth*, *pmr*, *P-31 nmr*)
Kolodyazhnyi, O.I. *et al*, *Tet. Lett.*, 1989, **30**, 2445 (*tetraisopropyl*, *synth*, *pmr*, *cmr*, *P-31 nmr*)
Kolodyazhnyi, O.I., *Zh. Obshch. Khim.*, 1990, **60**, 1727; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1990, **60**, 1541 (*tetraisopropyl*, *synth*, *P-31 nmr*)

5-(Chloromethyl)-2-pyrrolidinethione, 9CI C-1-00125



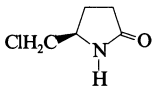
C_5H_8ClNS M 149.6

(*S*)-*form* [163230-53-3]
Cryst. solid ($CHCl_3$/hexane). Mp 126-128°. $[\alpha]_D$ −36.2 (c, 0.051 in $CHCl_3$).

Smith, D.C. *et al*, *J.O.C.*, 1995, **60**, 2692 (*synth*, *ir*, *pmr*, *ms*)

5-(Chloromethyl)-2-pyrrolidinone C-1-00126

[99382-20-4]



(*R*)-*form*

C_5H_8ClNO M 133.5

(*R*)-*form* [138541-53-4]
Solid. Mp 35° approx. $Bp_{0.1}$ 128°. $[\alpha]_D^{20}$ +1.6 (c, 2.5 in EtOH).

(*S*)-*form* [72479-04-0]
Solid. Mp 53-55°. $Bp_{0.15}$ 106.5-107°. $[\alpha]_D^{20}$ −18 (c, 2.5 in EtOH).

Silverman, R.B. *et al*, *J.O.C.*, 1980, **45**, 815 (*synth*)
Valasinas, A. *et al*, *J.O.C.*, 1992, **57**, 2158 (*synth*)

1-(Chloromethyl)-4-(trifluoromethyl)benzene C-1-00127

α′-*Chloro*-α,α,α-*trifluoro*-p-*xylene.* p-*Trifluoromethylbenzyl chloride*

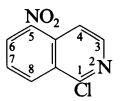
[939-99-1]

$C_8H_6ClF_3$ M 194.5
Mp 19°. Bp_{12} 68°. n_D^{22} 1.4622.

Streitwieser, A. *et al*, *J.A.C.S.*, 1964, **86**, 4938.

1-Chloro-5-nitroisoquinoline, 9CI C-1-00128

[58142-97-5]



$C_9H_5ClN_2O_2$ M 208.6
Cryst. Mp 187°.

Elpern, B. *et al*, *J.A.C.S.*, 1946, **68**, 1436 (*synth*)
Robinson, R.A. *et al*, *J.A.C.S.*, 1947, **69**, 1939 (*synth*)

3-Chloro-5-nitroisoquinoline, 9CI C-1-00129

[10296-47-6]

$C_9H_5ClN_2O_2$ M 208.6
Pale yellow needles (C_6H_6/hexane). Mp 163-165°.

Hall, C.E. *et al*, *Can. J. Chem.*, 1966, **44**, 2473 (*synth*)

4-Chloro-3-nitroisoquinoline C-1-00130

$C_9H_5ClN_2O_2$ M 208.6
Yellow needles (EtOH). Mp 108-109°.

Ikehara, M. *et al*, *Chem. Pharm. Bull.*, 1959, **7**, 501 (*synth*)

4-Chloro-5-nitroisoquinoline, C-1-00131
9CI

[53599-88-5]

$C_9H_5ClN_2O_2$ M 208.6
Pale yellow needles (EtOH aq.). Mp 180-182°.

Uff, B.C. *et al*, *J.C.S. Perkin 1*, 1974, 1146 (*synth, ir, pmr*)

5-Chloro-8-nitroisoquinoline, C-1-00132
9CI

[58142-95-3]

$C_9H_5ClN_2O_2$ M 208.6
Cryst. Mp 134-135°.

Manske, R.H.F. *et al*, *Can. J. Res., Sect. B*, 1949, **27**, 161; *CA*, **43**, 5783i (*synth*)

7-Chloro-8-nitroisoquinoline, C-1-00133
9CI

[78104-31-1]

$C_9H_5ClN_2O_2$ M 208.6
Cryst. Mp 146-147°.

Manske, R.H.F. *et al*, *Can. J. Res., Sect. B*, 1949, **27**, 161; *CA*, **43**, 5783i (*synth*)

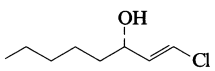
8-Chloro-5-nitroisoquinoline, C-1-00134
9CI

$C_9H_5ClN_2O_2$ M 208.6
Light yellow needles (MeOH). Mp 122-124°.

N-*Oxide:*
$C_9H_5ClN_2O_3$ M 224.6 Yellow needles. Mp 250-252° subl.

Wozniak, M. *et al*, *Annalen*, 1994, 355 (*synth, pmr*)

1-Chloro-1-octen-3-ol, 9CI C-1-00135



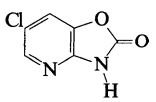
$C_8H_{15}ClO$ M 162.6
(*S*)-(*E*)-***form*** [116500-94-8]
Liq. $[\alpha]_D$ −4.8 (c, 4 in $CHCl_3$).

[67550-01-0, 116414-89-2, 132015-84-0, 168254-30-6]

Kitano, Y. *et al*, *Tet. Lett.*, 1987, **28**, 6351 (*synth*)
Yadav, J.S. *et al*, *Tet. Lett.*, 1990, **31**, 4495 (*synth*)
Yadav, J.S. *et al*, *Tetrahedron*, 1992, **48**, 4465 (*synth, pmr*)

6-Chlorooxazolo[4,5-*b*]pyridin-2(3*H*)-one, 9CI C-1-00136

[35570-68-4]



$C_6H_3ClN_2O_2$ M 170.5
Cryst. (EtOH aq.). Mp 188-189°.

Rüfenacht, K. *et al*, *Helv. Chim. Acta*, 1976, **59**, 1593 (*synth*)

Chloropentafluorobenzene, C-1-00137
9CI, 8CI

[344-07-0]

$(C_6F_5)Cl$

C_6ClF_5 M 202.5
Liq. d_4^{25} 1.568. Bp_{750} 122-123°.

Mcbee, E.T. *et al*, *Ind. Eng. Chem.*, 1947, **39**, 378 (*synth, props*)
Florin, R.E. *et al*, *J. Res. Natl. Bur. Stand. (U.S.)*, 1959, **62**, 1191 (*synth*)
Smithson, L.D. *et al*, *Org. Mass Spectrom.*, 1970, **4**, 1 (*ms*)
Obronravov, P.W.D. *et al*, *Zh. Org. Khim.*, 1977, **13**, 1679; *J. Org. Chem. USSR (Engl. Transl.)*, 1977, **13**, 1553 (*formn*)
Bardin, V.V. *et al*, *J. Fluorine Chem.*, 1983, **23**, 67 (*synth, F-19 nmr*)
Kinkead, E.R. *et al*, *Toxicol. Ind. Health*, 1990, **6**, 533; *CA*, **115**, 43966e (*tox*)
Zhukov, A.P. *et al*, *CA*, 1991, **115**, 268930p (*Cl-35 nqr, struct*)

2-Chloropentanal, 9CI C-1-00138

[41718-47-2]

$H_3CCH_2CH_2CHClCHO$

C_5H_9ClO M 120.5
(±)-***form***
Liq. Bp 126-130° (95% pure).

White, R.E. *et al*, *J.O.C.*, 1973, **38**, 3902 (*synth, ir, pmr*)
De Kimpe, N. *et al*, *Bull. Soc. Chim. Belg.*, 1992, **101**, 237 (*synth*)

4-Chloropentanal, 9CI C-1-00139
4-Chlorovaleraldehyde, 8CI

[17408-13-8]

$H_3CCHClCH_2CH_2CHO$

C_5H_9ClO M 120.5
(±)-***form***
Liq. Bp_{16} 70-71°.

Helferich, B. *et al*, *Ber.*, 1920, **53**, 2009 (*synth*)
Friederang, A.W. *et al*, *J.O.C.*, 1968, **33**, 3797 (*synth, ir, pmr*)

2-Chloro-3-pentanone, 9CI C-1-00140

[17042-21-6]

$H_3CCH_2COCHClCH_3$

C_5H_9ClO M 120.5
(±)-***form*** [117139-60-3]
Liq. Bp_{53} 60-61°, Bp_7 32-33°. n_D^{20} 1.4286.

Asinger, F. *et al*, *Annalen*, 1960, **634**, 164 (*synth*)
Wyman, D.P. *et al*, *J.O.C.*, 1964, **29**, 1956 (*synth, pmr*)
Ogloblin, K.A. *et al*, *Zh. Obshch. Khim.*, 1964, **34**, 1525; *J. Gen. Chem. USSR (Engl. Transl.)*, 1964, **34**, 1533 (*synth, ir*)
Gough, T.E. *et al*, *Can. J. Chem.*, 1967, **45**, 2529 (*synth, pmr*)
Föhlisch, B. *et al*, *Chem. Ber.*, 1986, **119**, 1661 (*cmr, ms*)
De Buyck, L. *et al*, *Bull. Soc. Chim. Belg.*, 1994, **103**, 21 (*pmr, cmr*)

3-Chloro-2-pentanone, 9CI C-1-00141

[13280-00-7]

$H_3CCH_2CHClCOCH_3$

C_5H_9ClO M 120.5
(±)-***form***
Liq. Bp_{745} 130-132°, Bp_{12} 36-38°. n_D^{20} 1.4280.

Oxime: [14352-56-8].
$C_5H_{10}ClNO$ M 135.5 Liq. Bp_{10} 75°.
▶ Lachrymator.

Buchman, E.R. *et al*, *J.A.C.S.*, 1945, **67**, 395 (*synth*)
Borrows, E.T. *et al*, *J.C.S.*, 1946, 1083 (*synth*)
Searles, S. *et al*, *J.O.C.*, 1957, **22**, 919 (*synth*)
Ogloblin, K.A. *et al*, *Zh. Obshch. Khim.*, 1964, **34**, 1525; *J. Gen. Chem. USSR (Engl. Transl.)*, 1964, **34**, 1533 (*synth, ir*)
Hart, H. *et al*, *J.A.C.S.*, 1968, **90**, 5189 (*synth, ir, ms, pmr*)
De Kimpe, N. *et al*, *Synthesis*, 1990, 595 (*synth*)

4-Chloro-2-pentanone, 9CI C-1-00142

[26386-83-4]

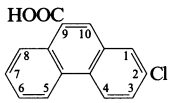
$H_3CCHClCH_2COCH_3$

C_5H_9ClO M 120.5
(±)-***form***
Oil. Bp 159-160°, Bp_{15} 48°.

Brown, E. *et al*, *Bull. Soc. Chim. Fr.*, 1972, 212 (*synth, pmr, ir*)

2-Chloro-9-phenanthrenecarboxylic acid C-1-00143

[56988-39-7]



$C_{15}H_9ClO_2$ M 256.6
Leaflets (EtOH aq.). Mp 240-242° (233-234°).

Schofield, K. *et al*, *J.C.S.*, 1949, 2393 (*synth*)
Wassmundt, F.W. *et al*, *J.O.C.*, 1995, **60**, 196 (*synth, ir, pmr*)

6-Chloro-9-phenanthrenecarboxylic acid C-1-00144

[56988-42-2]

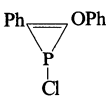
$C_{15}H_9ClO_2$ M 256.6
Needles (AcOH). Mp 301.5-302.5°.

Et ester:
$C_{17}H_{13}ClO_2$ M 284.7 Needles (EtOH). Mp 94.5-95°.

Nyler, P., *Ber.*, 1920, **53**, 158 (*synth, deriv*)
Wassmundt, F.W. *et al*, *J.O.C.*, 1995, **60**, 196 (*synth, pmr, ir*)

1-Chloro-2-phenoxy-3-phenyl-1*H*-phosphirene C-1-00145

[124946-31-2]



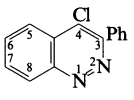
$C_{14}H_{10}ClOP$ M 260.6

Oil. $Bp_{0.002}$ 150° (oven).

Schnurr, W. *et al*, *Tet. Lett.*, 1989, **30**, 3951 (*synth, cmr, P-31 nmr*)

4-Chloro-3-phenylcinnoline C-1-00146

[13109-11-0]



$C_{14}H_9ClN_2$ M 240.6
Orange cryst. (Et_2O/petrol). Mp 119-120°.

Schofield, K. *et al*, *J.C.S.*, 1949, 2393 (*synth*)
Lowrie, H.S. *et al*, *J. Med. Chem.*, 1966, **9**, 670 (*synth*)
Vasilevsky, S.F. *et al*, *Synth. Commun.*, 1994, **24**, 1733 (*synth*)

6-Chloro-4-phenylcinnoline, 9CI C-1-00147

[21039-78-1]

$C_{14}H_9ClN_2$ M 240.6
Pale yellow needles (Et_2O/petrol). Mp 141-142°.

1-Oxide: [60794-31-2].
$C_{14}H_9ClN_2O$ M 256.6 Yellowish cryst. (CH_2Cl_2/petrol). Mp 195-197°.

2-Oxide: [60794-30-1].
$C_{14}H_9ClN_2O$ M 256.6 Pale yellow needles (CH_2Cl_2/MeOH). Mp 165-167°.

Bannore, S.N. *et al*, *Indian J. Chem.*, 1969, **7**, 654; 1973, **11**, 631 (*synth, ms*)
Walser, A. *et al*, *J. Het. Chem.*, 1976, **13**, 907 (*oxides*)

2-Chloro-3-phenyl-2-cyclobuten-1-one, 9CI C-1-00148

[91391-31-0]

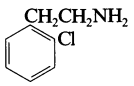
$C_{10}H_7ClO$ M 178.6
Long needles (petrol). Mp 67.8-69.2°.

Manatt, S.L. *et al*, *J.A.C.S.*, 1964, **86**, 2645 (*synth*)
Wiberg, K.B. *et al*, *J.A.C.S.*, 1993, **115**, 10645 (*synth*)

2-(2-Chlorophenyl)ethylamine C-1-00149

2-Chlorobenzeneethanamine, 9CI. 2-Chlorophenethylamine

[13078-80-3]



$C_8H_{10}ClN$ M 155.6
d 1.106. Bp_{15} 120°, Bp_3 94-95°. n_D^{20} 1.5516.

Hydrochloride: [18970-81-5].
Cryst. ($MeOH/Et_2O$). Mp 214-216°.

Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1282C.
Aldrich Library of NMR Spectra, **2**, 595C.
Price, R. *et al*, *Ann. Appl. Biol.*, 1978, **89**, 479 (*synth*)
Eur. Pat., 69 622, (1983); *CA*, **99**, 53332K.
Bompart, J. *et al*, *Ann. Pharm. Fr.*, 1987, **45**, 379 (*synth*)

2-(3-Chlorophenyl)ethylamine C-1-00150

3-Chlorobenzeneethanamine, 9CI. 3-Chlorophenethylamine

[13078-79-0]

$C_8H_{10}ClN$ M 155.6
Used in synthesis of $Ca^{2\oplus}$ entry blockers. Exhibits plant growth regulatory props. Liq. d 1.119. Bp_{12} 111-113°. n_D^{20} 1.5490.

Hydrochloride: [89042-13-7].
Cryst. ($MeOH/Et_2O$). Mp 157-160° dec.

Aldrich Library of FT-NMR Spectra, **2**, 601A.
Price, R. *et al*, *Ann. Appl. Biol.*, 1978, **89**, 479 (*synth*)
Hocquaux, M. *et al*, *Eur. J. Med. Chem.* (*Chim. Ther.*), 1983, **18**, 319; *CA*, **100**, 121427m (*synth*)
Carson, J.R. *et al*, *J. Med. Chem.*, 1988, **31**, 630 (*use*)

2-(4-Chlorophenyl)ethylamine C-1-00151

4-Chlorobenzeneethanamine, 9CI. 4-Chlorophenethylamine

[156-41-2]

$C_8H_{10}ClN$ M 155.6
Used in stimulation of sexual receptivity in the female rat. Liq. d 1.112. Bp_{16} 115-118°, Bp_{12} 124-129°. n_D^{20} 1.5480.

Hydrochloride: [2492-83-3].
Cryst. ($MeOH/Et_2O$). Mp 240-243° dec.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1172C.
Aldrich Library of NMR Spectra, 2nd edn., **1**, 1092C.
Wilson, C.A. *et al*, *Pharmacol., Biochem. Behav.*, 1982, **16**, 777; *CA*, **96**, 211162z (*pharmacol*)
Martin, I.L. *et al*, *Acta Cryst. B*, 1978, **34**, 2176 (*cryst struct*)
Price, R. *et al*, *Ann. Appl. Biol.*, 1978, **89**, 479 (*synth*)
Bennington, F. *et al*, *J.O.C.*, 1979, **23**, 1958 (*synth*)
Vejdelek, Z. *et al*, *Coll. Czech. Chem. Comm.*, 1990, **55**, 2345 (*synth*)
Caldwell, G.W. *et al*, *Org. Mass Spectrom.*, 1990, **25**, 317 (*ms*)

1-Chloro-7-phenylheptane C-1-00152

(7-Chloroheptyl)benzene, 9CI

[54636-29-2]

$Ph(CH_2)_6CH_2Cl$

$C_{13}H_{19}Cl$ M 210.7
Liq. Bp_2 129-132°.

Covant, J.B. *et al*, *J.A.C.S.*, 1924, **46**, 232 (*synth*)
Rossander, S.S. *et al*, *J.A.C.S.*, 1928, **50**, 1491 (*synth*)
Forth, M.A. *et al*, *J.O.C.*, 1994, **59**, 2616 (***synth***, *pmr*)

(Chlorophenylmethyl) phosphonic dichloride C-1-00153

α-Chlorobenzylphosphonic dichloride

[55691-59-3]

$PhCHClP(O)Cl_2$

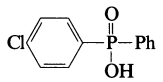
$C_7H_6Cl_3OP$ M 243.4

(±)-form
d_5^{40} 1.45. Mp 60-61° (48°). Bp_2 124-126°, $Bp_{0.3}$ 109°. n_D^{40} 1.5666.

Kabachnik, M.I. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1950, **75**, 219; *CA*, **45**, 6569 (*synth*)
Kinnear, A.M. *et al*, *J.C.S.*, 1952, 3437 (*synth*)
Miller, J.A. *et al*, *J.C.S. Perkin 1*, 1976, 535 (*synth, ir, pmr*)
Haiger, M.J.P. *et al*, *J.C.S. Perkin 1*, 1989, 563 (*pmr, P-31 nmr*)

(4-Chlorophenyl) phenylphosphinic acid C-1-00154

[13118-97-3]



$C_{12}H_{10}ClO_2P$ M 252.6
Solid. Mp 152-154°, Mp 158-160°.

2-Bromoethyl ester: [149794-62-7]. *2-Bromoethyl (4-chlorophenyl) phenylphosphinate*
Cryst. (hexane). Mp 78°.

Butyl ester: [41044-95-5]. *Butyl (4-chlorophenyl)phenylphosphinate*
$C_{16}H_{18}ClO_2P$ M 308.7 Oil. d_4^{20} 1.18. n_D^{20} 1.5642.

Chloride: [32395-30-5].
$C_{12}H_9Cl_2OP$ M 271.0 Liq. $Bp_{0.3}$ 155-157°. n_D^{20} 1.6169.

Azide:
$C_{12}H_9ClN_3OP$ M 277.6 Liq. $Bp_{0.01}$ 143-146°. n_D^{20} 1.6120.

Petrov, K.A. *et al*, *Zh. Obshch. Khim.*, 1973, **43**, 37; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1973, **43**, 34 (*ester, acid, synth*)
Weissbach, F. *et al*, *J. Prakt. Chem.*, 1975, **317**, 394 (*chloride, azide*)
Harger, M.I.P. *et al*, *J.C.S. Perkin 1*, 1985, 1787 (*synth, chloride*)
Neidlein, R. *et al*, *Monatsh. Chem.*, 1993, **124**, 309 (*synth, ms, ir, uv, pmr*)

2-Chloro-2-phenylpropane C-1-00155

(1-Chloro-1-methylethyl)benzene, 9CI. α-Chlorocumene, 8CI

[934-53-2]

$(H_3C)_2CClPh$

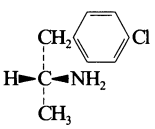
$C_9H_{11}Cl$ M 154.6
Oil. $Bp_{0.05}$ 37°. Dec. on distillation. n_D^{20} 1.5210.

Ross, H. *et al*, *Chem. Ber.*, 1956, **89**, 2641 (*synth*)
Jacot-Guillarmod, A., *Helv. Chim. Acta*, 1957, **40**, 1639 (*synth*)
Parham, W.E. *et al*, *J.O.C.*, 1981, **46**, 4804 (*synth, pmr*)
Gurudutt, K.N. *et al*, *Indian J. Chem., Sect. B*, 1993, **32**, 468 (*synth, pmr*)
Nölke, M. *et al*, *Annalen*, 1995, 41 (*synth, pmr*)

1-(4-Chlorophenyl)-2-propylamine C-1-00156

4-Chloro-α-methylbenzeneethanamine, 9CI. p-Chloro-α-methylphenethylamine. 4-Chloroamphetamine

[64-12-0]



(R)-form

$C_9H_{12}ClN$ M 169.6

Causes reversible short-term redn. in levels of 5-hydroxytryptamine and 5-hydroxyindoleacetic acid in brain conc.

(R)-form [405-47-0]

Hydrochloride: [16064-31-6]. $[\alpha]_D^{25}$ −22 (c, 2.16 in H_2O).

(S)-form [405-46-9]

Hydrochloride: [16064-30-5]. $[\alpha]_D^{25}$ +22.0 (c, 2.1 in H_2O), $[\alpha]_D^{25}$ −8.6 (c, 2.1 in 2-propanol).

(±)-form [2275-84-5]

$Bp_{0.2}$ 72°.

Hydrochloride: [3706-38-5]. Cryst. (EtOH/EtOAc/Et_2O). Mp 164-165°.

[25356-95-0]

Cavallini, G. *et al*, *Farmaco, Ed. Sci.*, 1956, **11**, 805 (*synth*)
Nielsen, C.K. *et al*, *Arch. Int. Pharmacodyn. Ther.*, 1967, **170**, 428 (*pharmacol*)
Smith, H.E. *et al*, *J. Med. Chem.*, 1974, **17**, 416 (*synth*)
Smith, H.E. *et al*, *J.O.C.*, 1975, **40**, 1562 (*synth, abs config*)
Foye, W.O. *et al*, *J. Pharm. Sci.*, 1979, **68**, 591 (*synth*)
Ames, M.M. *et al*, *Biochem. Pharmacol.*, 1982, **31**, 5 (*metab*)
Smith, H.E. *et al*, *J.A.C.S.*, 1983, **105**, 1578 (*synth, uv*)
Fuller, R.W., *Neurochem. Res.*, 1992, **17**, 449 (*rev*)

1-Chloro-2-propylamine C-1-00157

1-Chloro-2-propanamine, 9CI. 2-Chloro-1-methylethylamine, 8CI. β-Chloroisopropylamine

[37143-56-9]

$ClCH_2CH(NH_2)CH_3$

C_3H_8ClN M 93.5

(±)-form

Hydrochloride: Cryst. Mp 74-75°.

Coleman, G.H. *et al*, *J.A.C.S.*, 1928, **50**, 2739 (*synth*)
Minoura, Y. *et al*, *J.A.C.S.*, 1959, **81**, 4689 (*synth*)

2-Chloro-1-propylamine, 8CI C-1-00158

2-Chloro-1-propanamine, 9CI. 1-Amino-2-chloropropane

[14753-25-4]

$H_3CCHClCH_2NH_2$

C_3H_8ClN M 93.5

(±)-form

Hydrochloride: [6266-35-9]. Cryst. (EtOH). Mp 187-190° (180-181°).

[138373-82-7]

Jones, G.D. *et al*, *J.O.C.*, 1944, **9**, 125 (*synth*)
Schaefer, F.C. *et al*, *J.A.C.S.*, 1955, **77**, 5928 (*synth*)
Akerfeldt, S., *Acta Chem. Scand.*, 1966, **20**, 1783 (*synth*)

2-Chloro-2-propylphosphonic acid C-1-00159

(1-Chloro-1-methylethyl)phosphonic acid. α-Chloroisopropylphosphonic acid

$(H_3C)_2CClP(O)(OH)_2$

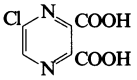
$C_3H_8ClO_3P$ M 158.5

Mono-Me ester: [110520-78-0]. $C_4H_{10}ClO_3P$ M 172.5 Solid (as anilinium salt). Mp 152-154° (anilinium salt).

Dichloride: [66794-41-0]. $C_3H_6Cl_3OP$ M 195.4 Solid. Mp 80° approx. $Subl._{1.5}$ 70°.

Harger, M.J.P. *et al*, *J.C.S. Perkin 1*, 1986, 1681 (*synth, ir, ms, pmr*)

5-Chloro-2,3-pyrazinedicarboxylic acid, 9CI C-1-00160



$C_6H_3ClN_2O_4$ M 202.5

Cryst. (dil. HCl) (as hydrochloride). Mp 199-202° dec. (hydrochloride).

Dinitrile: [72111-57-0]. *5-Chloro-2,3-dicyanopyrazine*
C_6HClN_4 M 164.5 Mp 89-90°.

Nakonwra, A. *et al*, *Agric. Biol. Chem.*, 1983, **47**, 2923 (*synth, nitrile*)
Obafemi, C.A. *et al*, *Helv. Chim. Acta*, 1994, **77**, 1549 (*synth, uv, pmr, cmr*)

2-Chloro-4-pyridinecarboxaldehyde, 9CI C-1-00161

2-Chloro-4-formylpyridine

[101066-61-9]

C_6H_4ClNO M 141.5

Eur. Pat., 183 369, (1986) (*Beecham*); *CA*, **105**, 97347r (*synth*)

4-Chloro-2-pyridinecarboxaldehyde, 9CI C-1-00162

4-Chloro-2-formylpyridine

[63071-13-6]

C_6H_4ClNO M 141.5

Mp 35-36°. $Bp_{0.5}$ 46°.

Furukawa, S., *J. Phys. Soc. Jpn.*, 1957, **77**, 11; *CA*, **51**, 8745g.
Schulz, O.E. *et al*, *Arch. Pharm. (Weinheim, Ger.)*, 1977, **310**, 128.

6-Chloro-3-pyridinecarboxaldehyde, 9CI C-1-00163

2-Chloro-5-formylpyridine. 6-Chloronicotinaldehyde

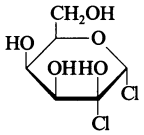
[23100-12-1]

C_6H_4ClNO M 141.5

Mp 71°.

Ziegler, F.E. *et al*, *Tet. Lett.*, 1969, 1097 (*synth*)
Vögtle, F. *et al*, *Synthesis*, 1994, 87 (*synth, pmr, ms, ir*)

2-*C*-Chlorotalopyranosyl chloride C-1-00164



$C_6H_{10}Cl_2O_5$ M 233.0

α-D-form

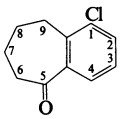
Tetrabenzoyl: [55628-80-3]. $C_{34}H_{26}Cl_2O_9$ M 649.4 Syrup. $[\alpha]_D^{25}$ +85.5 (c, 8.5 in $CHCl_3$).

Lundt, I. *et al*, *Acta Chem. Scand., Ser. B*, 1975, **29**, 70 (*tetrabenzoyl, cmr, pmr*)

1-Chloro-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one, 9CI C-1-00165

6-Chloro-1-benzosuberone

[21413-75-2]



$C_{11}H_{11}ClO$ M 194.6

Liq. Bp_{15} 162-165°. n_D^{20} 1.5764.

Oxime: [21413-76-3]. $C_{11}H_{12}ClNO$ M 209.6 Mp 136-138°.

Granger, R. *et al*, *C. R. Hebd. Seances Acad. Sci.*, 1961, **252**, 1478 (*synth*)
U.S. Pat., 3 632 853, (1972); *CA*, **77**, 5444x (*synth*)

2-Chloro-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one C-1-00166

7-Chloro-1-benzosuberone

[24127-36-4]

$C_{11}H_{11}ClO$ M 194.6

Liq. $Bp_{0.35}$ 110-113°.

Oxime: [24127-37-5]. $C_{11}H_{12}ClNO$ M 209.6 Needles (EtOH). Mp 128-131°.

Jones, D.H. *et al*, *J.C.S.(C)*, 1969, 2176 (*synth*)

3-Chloro-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one, 9CI C-1-00167

8-Chloro-1-benzosuberone

[21413-77-4]

$C_{11}H_{11}ClO$ M 194.6

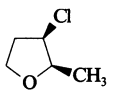
Mp 36-40°. $Bp_{2.9}$ 143-146°.

Oxime: [21413-78-5]. $C_{11}H_{12}ClNO$ M 209.6 Mp 139-141°.

Jones, D.H. *et al*, *J.C.S.(C)*, 1969, 2176 (*synth*)
U.S. Pat., 3 632 853, (1972); *CA*, **77**, 5444x (*synth*)

3-Chlorotetrahydro-2-methylfuran C-1-00168

3-Chloro-2-methyltetrahydrofuran



(2*RS*,3*RS*)-*form*

C_5H_9ClO M 120.5

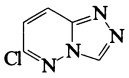
(2RS,3RS)-form
(±)-cis-*form*
Bp 146-147°.

(2RS,3SR)-form
Bp 132-134°.

Crombie, L. *et al*, *J.C.S. Perkin 1*, 1985, 1971; 1994, 673.

6-Chloro[1,2,4]triazolo[4,3-*b*] pyridazine C-1-00169

[28593-24-0]



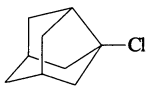
$C_5H_3ClN_4$ M 154.5
Needles. Mp 204-205°.

Sunder, S. *et al*, *J. Het. Chem.*, 1980, **17**, 1527 (*synth*)
Holyer, W. *et al*, *J. Het. Chem.*, 1995, **32**, 1341 (*synth, pmr, cmr*)

3-Chlorotricyclo[3.3.1.0^{3,7}] nonane C-1-00170

3-Chlorononoradamantane. 3a-Chlorooctahydro-2,5-methanopentalene, 9CI

[151697-49-3]



$C_9H_{13}Cl$ M 156.6
Cryst. Mp 121°.

Olah, G.A. *et al*, *J.A.C.S.*, 1993, **115**, 10728 (*synth, ms, pmr, cmr*)

13-Chloro-1-tridecanol C-1-00171

[72848-19-2]

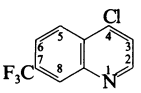
$ClCH_2(CH_2)_{11}CH_2OH$

$C_{13}H_{27}ClO$ M 234.8
Mp 47-48°.

Zakharkin, L.I. *et al*, *Zh. Org. Khim.*, 1981, **17**, 755; *J. Org. Chem. USSR (Engl. Transl.)*, 1981, **17**, 658 (*synth*)

4-Chloro-7-(trifluoromethyl) quinoline, 9CI C-1-00172

[346-55-4]



$C_{10}H_5ClF_3N$ M 231.6
Stabiliser for enzyme assay reagents. Cryst. (MeOH). Mp 71-72°.

N-*Oxide:* [55121-98-7].
$C_{10}H_5ClF_3NO$ M 247.6 Syrup.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1568B.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 733C.
Snyder, H.R. *et al*, *J.A.C.S.*, 1947, **69**, 371 (*synth*)
Ger. Pat., 2 428 194, (1975); *CA*, **82**, 171059y (*oxide*)

4-Chloro-8-(trifluoromethyl) quinoline, 9CI, 8CI C-1-00173

[23779-97-7]

$C_{10}H_5ClF_3N$ M 231.6
Cryst. (petrol). Mp 80-82° (78°).

Aldrich Library of FT-NMR Spectra, **3**, 427B.
Ger. Pat., 1 925 607, (1971); *CA*, **74**, 76341k.

Cholamine C-1-00174

*2-Amino-*N,N,N-*trimethylethanaminium(1+), 9CI*

[38170-37-5]

$H_2NCH_2CH_2NMe_3^{\oplus}$

$C_5H_{15}N_2^{\oplus}$ M 103.1 (ion)

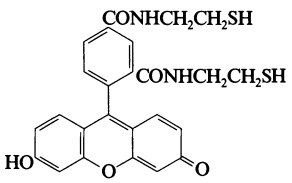
[10256-43-6, 53759-29-8, 130150-78-6]

Gabriel, S., *Ber.*, 1920, **53**, 1985 (*synth*)

Crabescein C-1-00175

*4-(6-Hydroxy-3-oxo-3*H*-xanthen-9-yl)-*N,N′-*bis(2-mercaptoethyl)-1,3-benzenedicarboxamide, 9CI*

[102072-98-0]



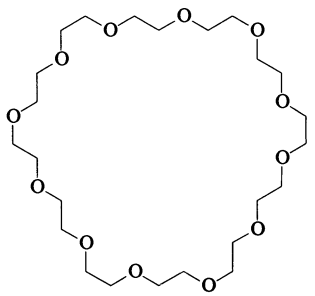
$C_{25}H_{22}N_2O_5S_2$ M 494.5
Labelling reagent. Links fluorescein to proteins across a disulfide bridge.

Packard, B. *et al*, *Biochemistry*, 1986, **25**, 3548 (*synth, uv, pmr, activity*)
Eur. Pat., 224 120, (1987) (*John Hopkins Univ*); *CA*, **108**, 18858 (*synth, use*)

36-Crown-12 C-1-00176

1,4,7,10,13,16,19,22,25,28,31,34-Dodecaoxacyclohexatriacontane, 9CI

[71092-59-6]



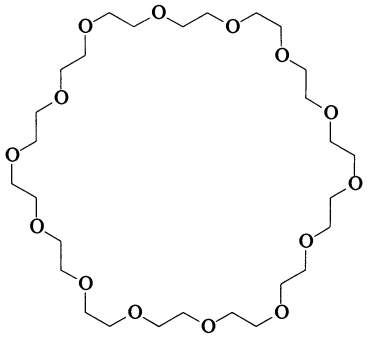
$C_{24}H_{48}O_{12}$ M 528.6
Cryst. (EtOH at −20°). Mp 54.5-57°.

Gibson, H.W. *et al*, *J.O.C.*, 1994, **59**, 2186 (*synth, ir, pmr, cmr, ms*)

42-Crown-14 C-1-00177

1,4,7,10,13,16,19,22,25,28,31,34,37,40-Tetradecaoxacyclodotetracontane, 9CI

[71092-60-9]



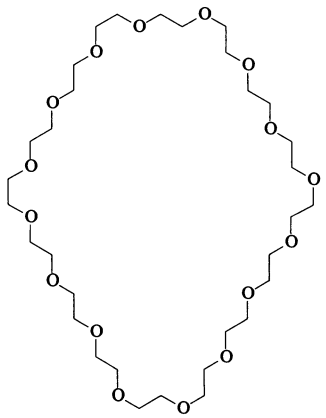
$C_{28}H_{56}O_{14}$ M 616.7
Cryst. (Me_2CO). Mp 55-57°.

Gibson, H.W. *et al*, *J.O.C.*, 1994, **59**, 2186 (*synth, ir, pmr, cmr, ms*)

48-Crown-16 C-1-00178

1,4,7,10,13,16,19,22,25,28,31,34,37,40,43,46-Hexadecaoxacyclooctatetracontane, 9CI

[71092-61-0]



$C_{32}H_{64}O_{16}$ M 704.8
Cryst. (Me_2CO). Mp 49.5-51°.

Gibson, H.W. *et al*, *J.O.C.*, 1994, **59**, 2186 (*synth, ir, pmr, cmr, ms*)

60-Crown-20 C-1-00179

1,4,7,10,13,16,19,22,25,28,31,34,37,40,43,46,49,52,55,58-Eicosaoctacyclohexacontane, 9CI

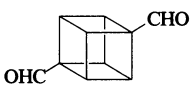
[71092-63-2]

$C_{40}H_{80}O_{20}$ M 881.0
Cryst. (Me_2CO). Mp 57-58°.

Gibson, H.W. *et al*, *J.O.C.*, 1994, **59**, 2186 (*synth, ir, pmr, cmr, ms*)

1,4-Cubanedicarboxaldehyde C-1-00180

1,4-Diformylcubane



$C_{10}H_8O_2$ M 160.1
Cryst. (hexane). Mp 133-135°.

Eaton, P.E. *et al*, *J.A.C.S.*, 1994, **116**, 7588 (*synth, pmr, cmr*)

Cyanodithioformic acid, 8CI C-1-00181

Carbonocyanidodithioic acid, 9CI

[38093-84-4]

NCC(S)SH

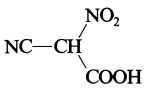
C_2HNS_2 M 103.1
Grey cryst. (H_2O). Mp 110° dec. Turns brown on standing.

Me ester: [17008-22-9]. *Methyl cyanodithioformate*
$C_3H_3NS_2$ M 117.1 Undergoes ene reactions with alkenes. Deep purple liq. Bp_1 50-60°.

Bähr, G. *et al*, *Ber.*, 1957, **90**, 438 (*synth*)
Simmons, H.E. *et al*, *J.A.C.S.*, 1962, **84**, 4786 (*Me ester*)
Vyas, D.M. *et al*, *Can. J. Chem.*, 1971, **49**, 3755.
Bray, J. *et al*, *Inorg. Synth.*, 1971, **13**, 187 (*synth*)
Vyas, D.M. *et al*, *J.C.S. Perkin 1*, 1975, 180.
Snider, B.B. *et al*, *J.A.C.S.*, 1976, **98**, 7115.
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, **7**, 237.
Kibbel, H.U. *et al*, *Z. Chem.*, 1981, **21**, 121 (*rev, synth, derivs*)

Cyanonitroacetic acid, 9CI C-1-00182

[166526-77-8]



$C_3H_2N_2O_4$ M 130.0
Salts exist in *aci*-nitro-form.

Di-Na salt: Disodium cyano-aci-*nitroacetate*
Pale yellow solid. Mp >300°.

Diammonium salt: Diammonium cyano-aci-*nitroacetate*
Pale yellow solid. Mp 120-137°.

Et ester:
$C_5H_6N_2O_4$ M 158.1 Cryst. (as K salt). Mp 240° (K salt).

Conrad, M. *et al*, *Ber.*, 1909, **42**, 735 (*ester*)
Nishiwaki, N. *et al*, *J. Het. Chem.*, 1995, **32**, 473 (*salts*)

P-Cyano-*N*,*N*,*N'*,*N'*-tetraisopropylphosphonous diamide C-1-00183

P-*Cyano*-N,N,N',N'-*tetrakis*(*1-methylethyl*) *phosphonous diamide*

[97135-49-4]

$[[(H_3C)_2CH]_2N]_2PCN$

$C_{13}H_{28}N_3P$ M 257.3
Solid. Mp 105°. $Bp_{0.01}$ 80-85°.

Igau, A. *et al*, *J.A.C.S.*, 1988, **110**, 6463 (*synth, pmr, P-31 nmr*)
Roques, C. *et al*, *J.O.C.*, 1989, **54**, 5535 (*synth, ms, pmr, P-31 nmr*)

Cyazone C-1-00184

Cyanoacetic acid 1-methylethylidene hydrazide, 9CI. Cyanoacetic acid isopropylidenehydrazide, 8CI

[4974-42-9]

$(H_3C)_2C{=}NNHCOCH_2CN$

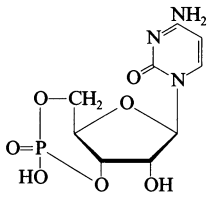
$C_6H_9N_3O$ M 139.1
Used in control of Dictyocaulus in sheep. Needles (Me_2CO). Mp 147-148°.

Zommer, S., *Acta Pol. Pharm.*, 1971, **28**, 14 (*synth, uv*)
Hamad, M.M., *Arch. Pharm.* (*Weinheim, Ger.*), 1990, **323**, 595 (*synth*)

Cyclic CMP C-1-00185

Cytidine cyclic 3',5'-(hydrogen phosphate), 9CI. Cyclic 3',5'-cytidylic acid

[3616-08-8]



$C_9H_{12}N_3O_7P$ M 305.1
λ_{max} 279 (ε 12430) (pH 2), 272 nm (9340) (H_2O, pH 7).

Na salt: [54925-33-6].
Solid + H_2O. λ_{max} 280 (ε 13650) (H_2O, pH 2), 272 nm (9550) (pH 7).

Ammonium salt: [55727-00-9].
Solid.

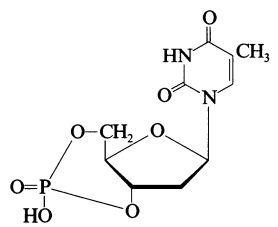
[108464-51-3]

Smith, M.S. *et al*, *J.A.C.S.*, 1961, **83**, 698 (*synth, uv*)
Ito, M. *et al*, *Agric. Biol. Chem.*, 1974, **38**, 2081 (*synth*)
Kainosho, M. *et al*, *J.A.C.S.*, 1975, **97**, 6839 (*conformn, pmr*)
Wierenga, W. *et al*, *J. Carbohydr., Nucleosides, Nucleotides*, 1977, **4**, 189 (*synth, uv, deriv*)
Baraniak, J. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1982, **56**, 441 (*synth, pmr*)
Beres, J. *et al*, *J. Med. Chem.*, 1985, **28**, 418 (*synth*)
Baraniak, J. *et al*, *J.C.S. Perkin 1*, 1987, 1645 (*synth*)
Newton, R.P. *et al*, *Nucleosides Nucleotides*, 1990, **9**, 365 (*ms*)

Cyclic TMP C-1-00186

Thymidine cyclic 3',5'-(hydrogen phosphate), 9CI. Cyclic 3',5'-thymidylic acid

[6453-60-7]



$C_{10}H_{13}N_2O_7P$ M 304.1
λ_{max} 260 nm (ε 10000) (H_2O, pH 7).

Na salt: [76567-90-3].
Solid.

Ammonium salt: [119999-00-7].
Solid.

Me ester: [120056-31-7]. *Thymidine cyclic 3',5'-(methylphosphate)*
$C_{11}H_{15}N_2O_7P$ M 318.2 Solid. Mp 92-102°.

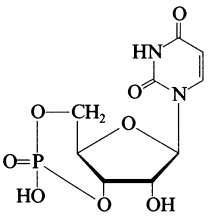
[120056-30-6]

Tener, G.M. *et al*, *J.A.C.S.*, 1958, **80**, 6223 (*synth, uv*)
Furusawa, K. *et al*, *J.C.S. Perkin 1*, 1976, 1711 (*synth, uv*)
Kainosho, M., *Org. Magn. Reson.*, 1979, **12**, 548 (*cmr*)
Japan. Pat., 80 120 793, (1980); *CA*, **94**, 137816f (*manuf*)
Ramos, D.L. *et al*, *J. Chromatogr.*, 1983, **261**, 83 (*hplc*)
Bentrude, W.G. *et al*, *J.A.C.S.*, 1989, **111**, 3981 (*synth*)
Broeders, N.L.H.L. *et al*, *J.A.C.S.*, 1990, **112**, 7475 (*synth, P-31 nmr, deriv*)
Newton, R.P. *et al*, *Nucleosides Nucleotides*, 1990, **9**, 365 (*ms*)

Cyclic UMP C-1-00187

Uridine cyclic 3',5'-(hydrogen phosphate), 9CI. Cyclic-3',5'-uridylic acid

[4004-57-3]



$C_9H_{11}N_2O_8P$ M 306.1
λ_{max} 260 nm (ε 10000) (H_2O, pH 7).

Ammonium salt: Solid + $2H_2O$.

Triethylammonium salt: Cryst. (EtOH/Et_2O or MeOH). Mp 220-223° dec. λ_{max} 261 (ε 9940) (pH 7), 260 nm (7740) (H_2O, pH 12).

Me ester: [56883-43-3].
$C_{10}H_{13}N_2O_8P$ M 320.1 Powder (dioxan).

Benzyl ester: [56942-15-5].
$C_{16}H_{17}N_2O_8P$ M 396.2 Powder.

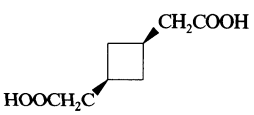
2'-Ac: [7390-55-8].
$C_{11}H_{13}N_2O_9P$ M 348.2 Cryst. (EtOH) (as triethylammonium salt). Mp 245° dec. (triethylammonium salt).

2'-Benzoyl: [52301-27-6].
$C_{16}H_{15}N_2O_9P$ M 410.2 λ_{max} 262 nm (MeOH).

[56942-13-3]

Smith, J. *et al*, *J.A.C.S.*, 1961, **83**, 698; 1959, **81**, 2911 (*synth, uv, deriv*)
Cozzone, P.J. *et al*, *Biochemistry*, 1976, **15**, 4853 (*P-31 nmr*)
Engels, J. *et al*, *Chem. Ber.*, 1977, **110**, 2 (*synth, pmr, deriv*)
Uesugi, S. *et al*, *Org. Magn. Reson.*, 1979, **12**, 143 (*cmr*)
Wang, X. *et al*, *CA*, 1980, **94**, 140088a (*synth*)
Zheng, Q. *et al*, *CA*, 1981, **30**, 1369 (*cryst struct*)
Baraniak, J. *et al*, *J.C.S. Perkin 1*, 1987, 1645 (*benzoyl*)
Newton, R.P. *et al*, *Nucleosides Nucleotides*, 1990, **9**, 365 (*ms*)
Perrett, D. *et al*, *Biomed. Chromatogr.*, 1991, **5**, 207; *CA*, **115**, 251308u (*hplc*)

1,3-Cyclobutanediacetic acid C-1-00188



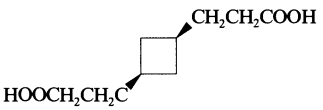
$C_8H_{12}O_4$ M 172.1

(1RS,3SR)-form
cis-*form*

Plates (H_2O). Mp 154.5-155.5°.

Paquette, L.A. *et al*, *J.O.C.*, 1994, **59**, 5700 (*synth*, *ir*, *pmr*, *cmr*)

1,3-Cyclobutanedipropanoic acid C-1-00189



$C_{10}H_{16}O_4$ M 200.2

(1RS,3SR)-form

cis-*form*

Flakes (H_2O). Mp 112.0-112.5°.

Di-Me ester:

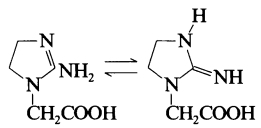
$C_{12}H_{20}O_4$ M 228.2 Oil.

Paquette, L.A. *et al*, *J.O.C.*, 1994, **59**, 5700 (*synth*, *ir*, *pmr*, *cmr*)

Cyclocreatine C-1-00190

2-Amino-4,5-dihydro-1H-imidazole-1-acetic acid, *9CI*. *2-Imino-1-imidazolidineacetic acid*. *1-(Carboxymethyl)-2-iminoimidazolidine*

[35404-50-3]



$C_5H_9N_3O_2$ M 143.1

Substrate for creatine kinase *in vitro*.

3-Phosphate: [61839-19-8]. *1-(Carboxymethyl)-2-imino-3-phosphonoimidazolidine*

$C_5H_{10}N_3O_5P$ M 223.1 Source of high energy phosphate. Stored in muscle, heart and brain.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **1**, 1329B (*nmr*)

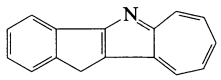
Struve, G.E. *et al*, *J.O.C.*, 1977, **42**, 4035 (*synth*, *cmr*, *struct*)

Woznicki, D.T. *et al*, *J. Neurochem.*, 1979, **33**, 75 (*formn*)

Phillips, G.N. *et al*, *J.A.C.S.*, 1979, **101**, 7120 (*bibl*, *cryst struct*, *phosphate*)

Roberts, J.J. *et al*, *Arch. Biochem. Biophys.*, 1983, **220**, 563 (*activity*)

11*H*-Cyclohepta[*b*]indeno[2,1-*d*]pyrrole C-1-00191

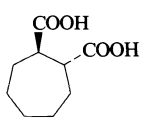


$C_{16}H_{11}N$ M 217.2

Reddish-violet needles. Mp 184-185°. pK_a 6.2 (MeCN/ aq. buffer).

Nitta, M. *et al*, *J.C.S. Perkin 1*, 1994, 2721 (*synth*, *pmr*, *cmr*)

1,2-Cycloheptanedicarboxylic acid, 9CI C-1-00192



(1*RS*,2*RS*)-*form*

$C_9H_{14}O_4$ M 186.2

(1RS,2RS)-form [6070-46-8]

(±)-trans-*form*

Cryst. (MeCN). Mp 158°. pK_{a1} 4.30; pK_{a2} 6.18 (25°).

Di-Me ester: [38312-28-6].

$C_{11}H_{18}O_4$ M 214.2 Bp_{10} 140-141°, $Bp_{0.5}$ 78°.

Di-Et ester:

$C_{13}H_{22}O_4$ M 242.3 Bp_9 149-150°, $Bp_{0.2}$ 80°.

Dinitrile: 1,2-Dicyanocycloheptane

$C_9H_{12}N_2$ M 148.2 $Bp_{0.7}$ 126-130°.

(1RS,2SR)-form [3603-86-9]

cis-*form*

Cryst. (Et_2O/methylcyclohexane). Mp 133-135°. pK_a 3.87 and 7.60 (25°).

Di-Me ester: [38312-27-5].

$Bp_{0.4}$ 85°, Bp_{15} 143-144°.

Anhydride: [4432-22-8]. *Hexahydro-1H-cyclohepta[c]furan-1,3-(3aH)-dione*, *9CI*

$C_9H_{12}O_3$ M 168.1 Cryst. (hexane/Et_2O). Mp 50-52°. $Bp_{0.5}$ 126-127°, $Bp_{0.25}$ 94°.

Ayres, D.C. *et al*, *J.C.S.*, 1958, 1779 (*synth*, *resoln*)

Sicher, J. *et al*, *Coll. Czech. Chem. Comm.*, 1961, **26**, 262 (*synth*)

Brannock, K.C. *et al*, *J.O.C.*, 1963, **28**, 1464 (*synth*)

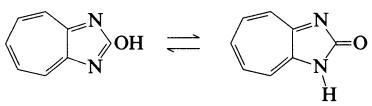
Svendsen, A. *et al*, *Tetrahedron*, 1973, **29**, 4251 (*synth*)

2(1*H*)-Cycloheptimidazolone, C-1-00193

9CI, 8CI

2-Hydroxycycloheptimidazole. *2-Cycloheptimidazolol*. *2-Hydroxy-1,3-diazaazulene*

[2132-33-4]



$C_8H_6N_2O$ M 146.1

Pale yellow needles (EtOH). Mp 245°.

NH-form

N-*Benzyl:* [363-13-3]. *1-(Phenylmethyl)-2(1H)-cycloheptimidazolone*, *9CI*. *1-Benzyl-2(1H)-cycloheptimidazolone*, *8CI*. ***Benhepazone, INN, JAN.*** *RCH 314*

$C_{15}H_{12}N_2O$ M 236.2 Analgesic. Antipyretic, antiinflammatory agent. Never marketed. Pale yellow cryst. (MeOH). Mp 181°.

▶ LD_{50} (mus, orl) 358 mg/kg. LD_{50} (mus, ipr) 119 mg/kg. GU4670500.

Nozoe, T. *et al*, *J.A.C.S.*, 1954, **76**, 3352 (*synth*)

Murata, I., *Bull. Chem. Soc. Jpn.*, 1960, **33**, 56 (*synth*)

Minakami, H. *et al*, *Life Sci.*, 1964, **3**, 305 (*pharmacol*)

Soma, N. *et al*, *Chem. Pharm. Bull.*, 1965, **13**, 819 (*benzyl*)

Murata, H. *et al*, *Chem. Pharm. Bull.*, 1967, **15**, 1906 (*anal*)

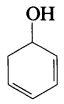
Takeshita, H. *et al*, *Heterocycles*, 1979, **12**, 653 (*cmr*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BEH000.

2,4-Cyclohexadien-1-ol, 9CI C-1-00194

Benzene hydrate

[66542-65-2]



C_6H_8O M 96.1

Liq. Bp_2 36-37°. Undergoes violent dec. on contact with acid, giving C_6H_6 and H_2O. Can be stored at −15° for several weeks.

▶ Potentially violent dec.

[77165-50-5]

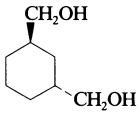
Stavascik, J. *et al*, *J.A.C.S.*, 1971, **93**, 3046 (*synth*, *ir*)

Rao, S.N. *et al*, *J.A.C.S.*, 1993, **115**, 5458 (*synth*, *uv*, *pmr*, *cmr*)

1,3-Cyclohexanedimethanol, 9CI C-1-00195

1,3-Bis(hydroxymethyl)cyclohexane

[3971-28-6]



(1*RS*,3*RS*)-*form*

$C_8H_{16}O_2$ M 144.2

(1RS,3RS)-form [13022-98-5]

(±)-trans-*form*

Liq. $Bp_{0.1}$ 112-114°.

(1RS,3SR)-form [5059-76-7]

cis-*form*

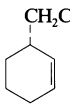
Cryst. (Et_2O). Mp 58°.

Haggis, G.A. *et al*, *J.C.S.*, 1953, 399 (*synth*)

Bridges, A.J. *et al*, *J.A.C.S.*, 1984, **106**, 1461 (*synth*, *pmr*)

2-Cyclohexene-1-acetic acid, 9CI C-1-00196

[3675-31-8]



(*R*)-*form*

$C_8H_{12}O_2$ M 140.1

(R)-form [133775-37-8]

Oil. $Bp_{0.6}$ 89-91°. $[\alpha]_D^{25}$ −51.1 (c, 0.52 in MeOH).

(S)-form [137174-05-1]

Oil. $[\alpha]_D^{27}$ +84.4 (c, 2.57 in $CHCl_3$).

(±)-***form*** [125973-24-2]

Oil. Mp 11°. Bp_{24} 150-152°. n_D^{25} 1.4787.

Nitrile: [82700-05-8]. *3-(Cyanomethyl) cyclohexene*

$C_8H_{11}N$ M 121.1 Bp_{15} 97°.

Mousseron, M. *et al*, *Bull. Soc. Chim. Fr.*, 1946, 604 (*synth*, *nitrile*)

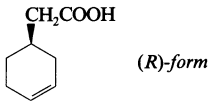
Blomquist, A.T. *et al*, *J.A.C.S.*, 1957, **79**, 4976 (*synth*)

Rosenmund, K.W. *et al*, *Chem. Ber.*, 1959, **92**, 486 (*synth*)

Takano, S. *et al*, *Synthesis*, 1994, 592 (*S-form*, *synth*, *ir*, *pmr*, *ms*)

3-Cyclohexene-1-acetic acid, 9CI C-1-00197

[10468-32-3]



(*R*)-*form*

$C_8H_{12}O_2$ M 140.1

(***R*)-*form*** [61362-44-5]
Liq. $Bp_{0.3}$ 92-94°. $[\alpha]_D^{26}$ +39.2 (neat).

Me ester: [67976-61-8].
$C_9H_{14}O_2$ M 154.2 Liq. Bp_7 72-75°. $[\alpha]_D^{26}$ +28.3 (neat).

Chloride:
$C_8H_{11}ClO$ M 158.6 Liq. Bp_{20} 95-96°. $[\alpha]_D^{21.5}$ +27.4 (c, 1.71 in CCl_4).

(±)-***form***
Liq. Bp_{25} 145-150°, $Bp_{0.1}$ 72°.

Me ester: Liq. Bp_{20} 90-05°.

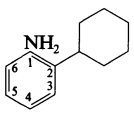
Nitrile: 4-(Cyanomethyl)cyclohexene
$C_8H_{11}N$ M 121.1 Liq. $Bp_{1.5}$ 62-64°.

Klein, J., *Isr. J. Chem.*, 1963, **1**, 385 (*synth, Me ester, nitrile*)
Doering, W. von E. *et al, J.A.C.S.*, 1972, **94**, 3833 (*synth, Me ester, chloride*)

2-Cyclohexylaniline C-1-00198

2-Aminophenylcyclohexane. 2-Amino-1′,2′,3′,4′,5′,6′-hexahydrobiphenyl

[4806-81-9]



$C_{12}H_{17}N$ M 175.2
Oil. Mp 13°. Bp_3 132-134°.

Hydrochloride: Needles (Et_2O). Mp 107.8°, Mp 172°.

N-*Ac:*
$C_{14}H_{19}NO$ M 217.3 Needles. Mp 101.2-102.0°.

Neunhoffer, O. *et al, J. Prakt. Chem.*, 1931, **133**, 95 (*synth*)
McGuine, T.H. *et al, J.A.C.S.*, 1947, **69**, 1469 (*synth*)
Rhoads, S.J. *et al, J.O.C.*, 1957, **22**, 321 (*synth, N-Ac*)
Harmata, M. *et al, Synthesis*, 1994, 142 (*ir, pmr, cmr*)

3-Cyclohexylaniline C-1-00199

3-Aminophenylcyclohexane. 3-Amino-1′,2′,3′,4′,5′,6′-hexahydrobiphenyl

[5369-21-1]

$C_{12}H_{17}N$ M 175.2
$Bp_{1.5}$ 123-125°.

Rhoads, S.J. *et al, J.O.C.*, 1957, **22**, 321 (*synth*)

4-Cyclohexylaniline C-1-00200

4-Aminophenylcyclohexane. 4-Amino-1′,2′,3′,4′,5′,6′-hexahydrobiphenyl

[6373-50-8]

$C_{12}H_{17}N$ M 175.2
Plates (EtOH aq.). Mp 55° (50.8-52.4°). $Bp_{0.3}$ 110-114°.

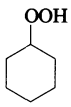
N-*Ac:* [29030-57-7]. N-(*4-Cyclohexylphenyl*) *acetamide, 9CI*
$C_{14}H_{19}NO$ M 217.3 Mp 131.4-131.9° (129°).

Mayes, H.A. *et al, J.C.S.*, 1929, 500 (*synth, N-Ac*)
Rhoads, S.J. *et al, J.O.C.*, 1957, **22**, 321 (*synth, N-Ac*)
Erickson, E.H. *et al, J. Med. Chem.*, 1979, **22**, 816 (*synth*)

Cyclohexyl hydroperoxide, 9CI, 8CI C-1-00201

Hydroperoxycyclohexane

[766-07-4]



$C_6H_{12}O_2$ M 116.1
$Bp_{0.08}$ 39-40°.

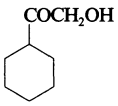
▶ Potentially explosive.

Aganov, A.V. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1982, 271 (*cmr*)
Pryor, W.A. *et al, J.O.C.*, 1985, **50**, 185 (*synth*)
Chernov, P.P. *et al, Zh. Org. Khim.*, 1986, **22**, 1883; *J. Org. Chem. USSR (Engl. Transl.)*, 1986, **22**, 1691 (*cmr, conformn*)
Brown, H.C. *et al, Tetrahedron*, 1987, **43**, 4059 (*synth*)
Druliner, J.D. *et al, J.O.C.*, 1988, **53**, 700 (*synth*)

1-Cyclohexyl-2-hydroxyethanone, 9CI C-1-00202

(Hydroxyacetyl)cyclohexane

[6004-53-1]



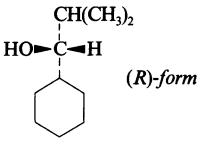
$C_8H_{14}O_2$ M 142.1
Oil. Bp_4 115-116°.

Matsumoto, T. *et al, J.O.C.*, 1985, **50**, 603 (*synth, ir, pmr, cmr*)
Fetizon, M. *et al, Tet. Lett.*, 1985, **26**, 3453 (*synth, ir, pmr, cmr*)
Ogawa, K. *et al, Chem. Pharm. Bull.*, 1987, **35**, 2426 (*synth, pmr*)

1-Cyclohexyl-2-methyl-1-propanol C-1-00203

α-(1-Methylethyl)cyclohexanemethanol, 9CI.
α-Isopropylcyclohexanemethanol, 8CI.
Cimepanol, INN. Bilidia

[29474-12-2]



(*R*)-*form*

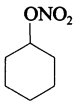
$C_{10}H_{20}O$ M 156.2
Sedative, analgesic, choleretic agent.

(***R*)-*form*** [156569-67-4]
Bp_{16} 98-101°. $[\alpha]_D^{24}$ −8.41 (neat).

Cram, D.J. *et al, J.A.C.S.*, 1959, **81**, 2737 (*synth*)
Burrows, E.P. *et al, J.A.C.S.*, 1960, **82**, 880 (*synth*)
Ota, M., *Yuki Gosei Kagaku Kyokaishi*, 1970, **28**, 762; *CA*, **73**, 98458 (*synth*)
Baldwin, J.E. *et al, Chem. Comm.*, 1984, 22 (*synth*)
Markó, I.E. *et al, Tetrahedron: Asymmetry*, 1994, **5**, 569 (*synth*)

Cyclohexyl nitrate C-1-00204

[2108-66-9]



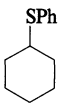
$C_6H_{11}NO_3$ M 145.1
Liq. d_4^{24} 1.0908. Bp 171°, Bp_3 52-53°. n_D^{19} 1.4565.

Kornblum, N. *et al, J.A.C.S.*, 1952, **74**, 3076 (*synth*)
Klochkov, V.V. *et al, Zh. Obshch. Khim.*, 1989, **59**, 1693; *J. Gen. Chem. USSR (Engl. Transl.)*, 1989, **59**, 1506 (*synth, conformn, cmr, ms*)
Olah, G.A. *et al, Synthesis*, 1993, 207 (*synth, cmr*)

Cyclohexyl phenyl sulfide, 8CI C-1-00205

(Cyclohexylthio)benzene, 9CI

[7570-92-5]



$C_{12}H_{16}S$ M 192.3
Oil. Bp_{12} 150-152°.

S-*Oxide:* see *Cyclohexyl phenyl sulfoxide, C-1-00206*

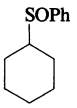
S,S-*Dioxide:* [6947-57-5]. *Cyclohexyl phenyl sulfone, 8CI. (Cyclohexylsulfonyl)benzene, 9CI*
$C_{12}H_{16}O_2S$ M 224.3 Cubes (MeOH); tablets (AcOH). Mp 76° (74°).

Cunneen, J.I., *J.C.S.*, 1947, 36 (*synth, dioxide*)
Weibull, B., *Ark. Kemi*, 1951, **3**, 171 (*dioxide, synth*)
Eliel, E.L. *et al, J.A.C.S.*, 1957, **79**, 5995 (*synth*)
Duddeck, H. *et al, Magn. Reson. Chem.*, 1986, **24**, 792 (*pmr, cmr, ir, ms*)
Fuchs, P.L. *et al, Synth. Commun.*, 1991, **21**, 1675 (*dioxide, synth*)
Olah, G.A. *et al, Synthesis*, 1992, 465 (*synth, cmr, ms*)

Cyclohexyl phenyl sulfoxide, 8CI C-1-00206

(Cyclohexylsulfinyl)benzene, 9CI

[3324-82-1]



$C_{12}H_{16}OS$ M 208.3

(±)-***form*** [94405-89-7]
Cryst. (petrol). Mp 64-65° (57.5-58.5°). Opt.-active forms not well descr.

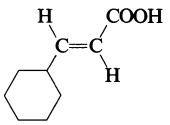
Weibull, B., *Ark. Kemi*, 1951, **3**, 171 (*synth*)
Eliel, E.L. *et al, J.O.C.*, 1965, **30**, 855 (*synth*)
Kice, J.L. *et al, J.O.C.*, 1967, **32**, 1631 (*synth*)

Duddeck, H. *et al*, *Magn. Reson. Chem.*, 1986, **24**, 792 (*pmr, cmr, ir, ms*)
Ghelfi, F. *et al*, *Synth. Commun.*, 1993, **23**, 1759; 1994, **24**, 2393 (*synth, pmr*)

3-Cyclohexyl-2-propenoic acid, 9CI C-1-00207

Cyclohexaneacrylic acid, 8CI

[4484-35-9]



(*E*)-*form*

$C_9H_{14}O_2$ M 154.2

(*E*)-*form* [56453-86-2]
Cryst. (hexane). Mp 57-58°. Bp_{11} 153-154°, $Bp_{0.3}$ 75°.

Me ester: [26429-99-2].
$C_{10}H_{16}O_2$ M 168.2 Bp_{15} 92-93°, $Bp_{0.3}$ 75°.

Et ester: [17343-88-3].
$C_{11}H_{18}O_2$ M 182.2 Bp_{11} 119°, Bp_2 57-58°.

Chloride: [52331-62-1].
$C_9H_{13}ClO$ M 172.6 Bp_{12} 142°.

Nitrile: [22031-57-8]. *1-Cyano-2-cyclohexylethylene*
$C_9H_{13}N$ M 135.2 Bp_4 85-86°.

(*Z*)-*form*

Nitrile: [78978-70-8].
Bp_7 110°.

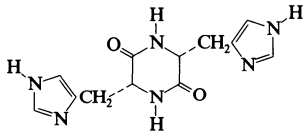
[6048-09-5]

Sircar, S.S.G., *J.C.S.*, 1928, 54.
Linstead, R.P. *et al*, *J.C.S.*, 1937, 1136.
Bestmann, H.J. *et al*, *Chem. Ber.*, 1970, **103**, 685 (*E-form, Me ester, ir*)
Larock, R.C., *J.O.C.*, 1975, **40**, 3236 (*E-form, Me ester*)
Outurquin, F. *et al*, *Synthesis*, 1989, 690 (*synth*)

Cyclo(histidylhistidyl) C-1-00208

3,6-Bis(1H-imidazol-4-ylmethyl)-2,5-piperazinedione, 9CI, 8CI

[6858-59-9]



(3*R*,6*R*)-*form*

$C_{12}H_{14}N_6O_2$ M 274.2

(*3R,6R*)-*form* [118139-79-0]
(+)-cis-*form*
Mp 288-292°. $[\alpha]_D$ +60 (c, 0.4 in 2*M* HCl).

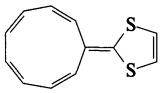
(*3S,6S*)-*form* [16944-59-5]
(−)-cis-*form*
Cryst. (H_2O). Mp 299-300° dec. $[\alpha]_D^{20}$ −60.5 (c, 1 in 1*M* HCl).

(*3RS,6SR*)-*form* [116051-89-9]
(±)-trans-*form*
Mp >280°. pK_{a1} 6.531; pK_{a2} 5.491.

Ziauddin, K.D. *et al*, *Tet. Lett.*, 1972, 483 (*pmr, uv*)
Oku, J. *et al*, *Makromol. Chem.*, 1979, **180**, 1089; 1982, **183**, 579 (*synth*)
Kojima, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1985, **58**, 409 (*cryst struct, pmr*)
Arena, G. *et al*, *Inorg. Chem.*, 1987, **26**, 795 (*synth*)
Jackson, W.R. *et al*, *Aust. J. Chem.*, 1988, **41**, 203 (*synth, pmr*)
Benedetti, E. *et al*, *Int. J. Pept. Protein Res.*, 1988, **31**, 220 (*trans, synth, uv, pmr, cryst struct*)

2-(2,4,6,8-Cyclononatetraen-1-ylidene)-1,3-dithiole C-1-00209

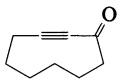
1,4-Dithianonapentafulvalene



$C_{12}H_{10}S_2$ M 218.3
Yellow oil.

Chai, S. *et al*, *Helv. Chim. Acta*, 1994, **77**, 1377 (*synth, uv, pmr, cmr, ms*)

2-Cyclononyn-1-one C-1-00210



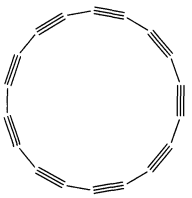
$C_9H_{12}O$ M 136.1
Liq. $Bp_{0.6}$ 120°.

Gleiter, R. *et al*, *Synthesis*, 1995, 969 (*synth, pmr, cmr, ir*)

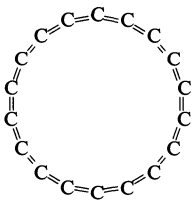
Cyclooctadecanonayne C-1-00211

Cyclo[18]carbon. Cyclooctadecaoctadecaene

[126487-09-0]



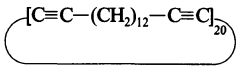
or



C_{18} M 216.1
Not yet known. 3 synthetic approaches tried. Representative of the unknown class of cyclo[*n*]carbon carbon valence isomers. Not known whether the ground state will be cyclopolyalkyne or cycloallene.

Diederich, F. *et al*, *Helv. Chim. Acta*, 1994, **77**, 1441.

1,3,25,27,49,51,73,75,97,99,121,123,145,147,169,171,193,195,217,241,243,265,267-Cyclooctaoctacontadohectatetracosayne C-1-00212

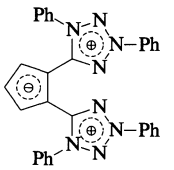


$C_{288}H_{480}$ M 3942.9

Conts. largest ring currently characterised (1995). Mp 112.5-115.5° (sinters at 111.5°).

Schill, G. *et al*, *Chem. Ber.*, 1978, **111**, 2901.

5,5′-(1,3-Cyclopentadiene-1,2-diyl)bis[1,3-diphenyl-1*H*-tetrazolium](1+), 9CI C-1-00213

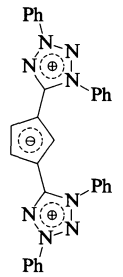


$C_{31}H_{23}N_8^{\oplus}$ M 507.5 (ion)
Tripolar mesoionic compd.

Trifluoromethanesulfonate: [170663-71-5].
$C_{32}H_{23}F_3N_8O_3S$ M 656.6 Red cryst. (EtOH/Et_2O). Mp 177°.

Araki, S. *et al*, *J.C.S. Perkin 1*, 1995, 1989 (*synth, ir, uv, cmr, pmr*)

5,5′-(1,3-Cyclopentadiene-1,3-diyl)bis[1,3-diphenyl-1*H*-tetrazolium](1+), 9CI C-1-00214

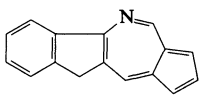


$C_{31}H_{23}N_8^{\oplus}$ M 507.5 (ion)
Tripolar mesoionic compd.

Trifluoromethanesulfonate: [170663-73-7].
$C_{32}H_{23}F_3N_8O_3S$ M 656.6 Yellow powder. Mp 145°.

Araki, S. *et al*, *J.C.S. Perkin 1*, 1995, 1989 (*synth, uv, ir, pmr, cmr*)

11*H*-Cyclopenta[*e*]indeno[1,2-*b*]azepine C-1-00215



$C_{16}H_{11}N$ M 217.2
Violet needles (EtOH). Mp 190°.

Nitta, M. *et al*, *J.C.S. Perkin 1*, 1995, 1001 (*synth, pmr, cmr, ir*)

3-Cyclopenten-1-amine, 9CI C-1-00216

3-Aminocyclopentene

[27721-59-1]

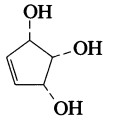
C_5H_9N M 83.1

Hydrochloride: [91469-55-5].
Cryst. (EtOH/Et_2O). Mp 219-221° (211-213°). Hygroscopic.

Murdock, K.C. *et al*, *J.O.C.*, 1962, **27**, 2395 (*synth*)
Elliot, R.D. *et al*, *J. Med. Chem.*, 1994, **37**, 739 (*synth, pmr*)

4-Cyclopentene-1,2,3-triol C-1-00217

[56772-30-6]



(1α,2α,3α)-*form*

$C_5H_8O_3$ M 116.1
3 Stereoisomers possible.

(*1α,2α,3α*)-***form*** [29782-84-1]
Needles (EtOAc). Mp 64-66°. *Meso-*.

Tribenzoyl:
$C_{26}H_{20}O_6$ M 428.4 Cryst. (EtOH). Mp 75°.

(*1α,2β,3α*)-***form*** [29782-82-9]
Constit. of *Ceratiosicyos laevis*. Prisms (Me_2CO). Mp 111°. *Meso-*.

Tribenzoyl: [4157-20-4].
Cryst. (EtOH). Mp 98°.

(*1α,2α,3β*)-***form*** [30276-77-8]
Prisms (petrol). Mp 67-68°. Racemate.

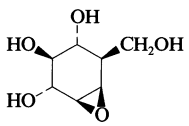
Tribenzoyl: [30276-78-9].
Cryst. (EtOH). Mp 76-77°.

Gaoni, Y. *et al*, *Bull. Soc. Chim. Fr.*, 1959, 705 (*synth*)
Wolczunowicz, G. *et al*, *Helv. Chim. Acta*, 1970, **53**, 1511, 2275; 1971, **54**, 1676 (*synth, pmr*)
Singy, G.A. *et al*, *Helv. Chim. Acta*, 1974, **57**, 1158 (*ms*)
Jensen, S.R. *et al*, *Phytochemistry*, 1986, **25**, 2349 (*isol*)
Begley, M.J. *et al*, *J.C.S. Perkin 1*, 1992, 57 (*synth, pmr*)

Cyclophellitol C-1-00218

3,4,5-Trihydroxy-7-oxabicyclo[4.1.0]heptane-2-methanol. 2,3-Epoxy-4,5,6-trihydroxy-1-cyclohexanemethanol. 1,2-Anhydro-3-deoxy-3-(hydroxymethyl)-D-myo-inositol

[126661-83-4]



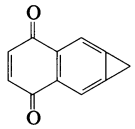
Absolute configuration

$C_7H_{12}O_5$ M 176.1
Isol. from a mushroom, *Phellinus* sp. β-Glucosidase inhibitor. Plates (H_2O). Mp 149-151°. $[\alpha]_D^{27}$ +103 (c, 0.5 in H_2O).

Atsumi, S. *et al*, *J. Antibiot.*, 1990, **43**, 49, 1579 (*isol, pmr, cmr, cryst struct, props*)
Tatsuta, K. *et al*, *Tet. Lett.*, 1990, **31**, 1171 (*synth*)
Tatsuta, K. *et al*, *J. Antibiot.*, 1991, **44**, 456 (*synth, props*)
Moritz, V. *et al*, *Tet. Lett.*, 1992, **33**, 5243 (*synth*)
Akiyama, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1993, **66**, 3760 (*synth*)
Shing, T.K.M. *et al*, *J.C.S. Perkin 1*, 1994, 2017 (*synth, pmr*)
McDevitt, R.E. *et al*, *J.O.C.*, 1994, **59**, 3250 (*synth*)

1*H*-Cyclopropa[*b*]naphthalene-3.6-dione, 9CI C-1-00219

[153202-81-4]



$C_{11}H_6O_2$ M 170.1
First stable cyclopropaquinone. Bright yellow needles (CH_2Cl_2/hexanes at −40°). Mp 130-132° dec.

Halton, B. *et al*, *J.C.S. Perkin 1*, 1993, 2239 (*synth, pmr, cmr*)

1,1-Cyclopropanediol, 9CI, 8CI C-1-00220

Cyclopropanone hydrate

[15144-65-7]

$C_3H_6O_2$ M 74.0
Mp 82-84°.

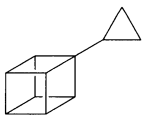
Di-Ac: [14743-57-8].
$C_7H_{10}O_4$ M 158.1 Cryst. (petrol). Mp 62-63°.

Grewe, R. *et al*, *Ber.*, 1963, **96**, 2819 (*synth*)
Schaafsma, S.E. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1967, **86**, 651 (*synth*)
van Tilborg, W.J.M. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1974, **93**, 290 (*synth*)

Cyclopropylcubane C-1-00221

Cyclopropylpentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane, 9CI

[134857-56-0]



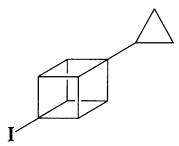
$C_{11}H_{12}$ M 144.2
Oil. Mp −31°.

Eaton, P.E. *et al*, *J.O.C.*, 1995, **60**, 966 (*synth, pmr, cmr*)

1-Cyclopropyl-4-iodocubane C-1-00222

1-Cyclopropyl-4-iodopentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane, 9CI

[161088-19-3]



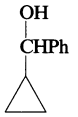
$C_{11}H_{11}I$ M 270.1
Cryst. powder. Mp 76.5-77.5°.

Eaton, P.E. *et al*, *J.O.C.*, 1995, **60**, 766 (*synth, pmr, cmr*)

Cyclopropylphenylmethanol C-1-00223

α-Cyclopropylbenzenemethanol, 9CI. α-Cyclopropylbenzyl alcohol, 8CI. Cyclopropylphenylcarbinol

[1007-03-0]



$C_{10}H_{12}O$ M 148.2
Bp_{12} 121°.

(±)-***form*** [63226-80-2]
Me ether: [5558-08-7].
Cyclopropylmethoxyphenylmethane
$C_{11}H_{14}O$ M 162.2 Bp_{33} 106-115°, Bp_{14} 94-95°.

[110548-55-5, 110548-56-6]

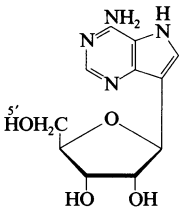
Olah, G.A. *et al*, *J.A.C.S.*, 1974, **96**, 3548 (*cmr*)
Baldry, P.J., *J.C.S. Perkin 1*, 1975, 1913 (*synth, ir, pmr*)
Hall, S.S. *et al*, *Chem. Ind. (London)*, 1976, 216 (*synth, pmr, ms*)
Pirkle, W.H. *et al*, *J.O.C.*, 1981, **46**, 2935 (*resoln*)
Dallinga, J.W. *et al*, *Org. Mass Spectrom.*, 1981, **16**, 183 (*ms*)
Leeper, F.J. *et al*, *Tet. Lett.*, 1989, **30**, 5017.

D

9-Deazaadenosine D-1-00001

1-C-(4-Amino-5H-pyrrolo[3,2-d]pyrimidin-7-yl)-1,4-dihydro-D-ribitol, 9CI

[77691-03-3]



$C_{11}H_{14}N_4O_4$ M 266.2

Isol. from the cyanobacterium *Anabaena affinis*. Cytotoxic agent.

Hydrochloride: [77699-40-2].
Cryst. (EtOH). Mp 179-183°.

5'-O-α-D-Glucopyranoside: [146445-11-6].
$C_{17}H_{24}N_4O_9$ M 428.3 Isol. from *A. affinis*. $[\alpha]_D^{28}$ +21.9 (c, 0.05 in H_2O).

[77699-39-9]

Lim, M.-I. *et al*, *Tet. Lett.*, 1981, **22**, 25 (*synth, pmr*)
Chu, M.Y. *et al*, *Biochem. Pharmacol.*, 1984, **33**, 1229 (*props*)
Namikoshi, M. *et al*, *J.A.C.S.*, 1993, **115**, 2504 (*isol, struct*)

3,8-Decadiyn-1-ol D-1-00002

[160109-64-8]

$H_3CC{\equiv}C(CH_2)_3C{\equiv}CCH_2CH_2OH$

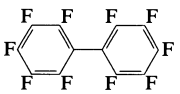
$C_{10}H_{14}O$ M 150.2
Oil.

Bao, J. *et al*, *J.A.C.S.*, 1994, **116**, 7616 (*synth, ir, pmr, cmr, ms*)

Decafluorobiphenyl D-1-00003

Perfluorobiphenyl

[434-90-2]

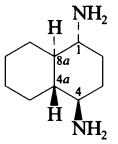


$C_{12}F_{10}$ M 334.1
Cryst. (C_6H_6). Mp 68-70°. Bp 206°, Bp_{20} 110°.

Nield, E. *et al*, *J.C.S.*, 1959, 166 (*synth*)
Brooke, G.M. *et al*, *J.C.S.*, 1964, 729 (*synth*)
Weidenbruch, M. *et al*, *Chem. Ber.*, 1972, **105**, 173 (*synth*)
Gleason, W.B. *et al*, *Cryst. Struct. Commun.*, 1976, **5**, 483 (*cryst struct*)
Arthur, J.W. *et al*, *J. Raman Spectrosc.*, 1976, **4**, 353 (*Raman*)
Matsumoto, H. *et al*, *J.O.C.*, 1983, **48**, 840 (*synth*)
Aroney, M.J. *et al*, *J. Mol. Struct.*, 1985, **127**, 175 (*conformn*)

Decahydro-1,4-naphthalenediamine, 9CI D-1-00004

1,4-Diaminodecalin. 1,4-Decalindiamine



(1*RS*,4*RS*,4a*RS*,8a*RS*)-*form*

$C_{10}H_{20}N_2$ M 168.2

(1RS,4RS,4aRS,8aRS)-form [20616-59-5]
(1α,4β,4aβ,8aα)-*form*
d^{20} 1.01. Mp 32-33.5°. Bp 90°. n_D^{20} 1.5201.

N,N'-*Di-Ac:* [20616-73-3].
$C_{14}H_{24}N_2O_2$ M 252.3 Mp 317-318°.

N,N'-*Dibenzoyl:* [20616-69-7].
$C_{24}H_{28}N_2O_2$ M 376.4 Mp 312-313°.

(1RS,4SR,4aRS,8aSR)-form [20616-62-0]
(1α,4α,4aβ,8aβ)-*form*
d^{20} 1.02. Mp 2-3°. Bp 88-90°. n_D^{20} 1.5218.

N,N'-*Dibenzoyl:* [20616-71-1].
Mp 218-219°.

(1RS,4SR,4aSR,8aRS)-form [20616-63-1]
(1α,4β,4aα,8aα)-*form*
d^{20} 1.02. Mp 39-40°. Bp 102-105°. n_D^{20} 1.523.

N,N'-*Di-Ac:* [20616-75-5].
Mp 328°.

N,N'-*Dibenzoyl:* [20616-72-2].
Mp 353-354°.

(1RS,4RS,4aSR,8aSR)-form [20616-61-9]
(1α,4β,4aα,8aβ)-*form*
d^{20} 0.99. Mp 26-27°. Bp 102° (approx.). n_D^{23} 1.5138.

N,N'-*Di-Ac:* [20616-74-4].
Mp 405-410°.

N,N'-*Dibenzoyl:* [21906-73-0].
Mp >360°.

(1RS,4SR,4aSR,8aSR)-form [20616-60-8]
d^{20} 1.00. Bp 100° (approx.). n_D^{20} 1.5157.

N,N'-*Dibenzoyl:* [20616-70-0].
Mp 228°.

Feltkamp, H. *et al*, *Arch. Pharm. (Weinheim, Ger.)*, 1986, **301**, 374 (*synth*)

Decahydro-1,5-naphthalenediamine D-1-00005

1,5-Diaminodecalin. 1,5-Decalindiamine

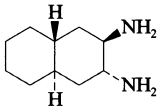
[40015-87-0]

$C_{10}H_{20}N_2$ M 168.2

Ger. Pat., 2 132 547, (1973); *CA*, **78**, 97193m.

Decahydro-2,3-naphthalenediamine D-1-00006

2,3-Diaminodecalin. 2,3-Decalindiamine



(2*RS*,3*RS*,4a*RS*,8a*RS*)-*form*

$C_{10}H_{20}N_2$ M 168.2

(2RS,3RS,4aRS,8aRS)-form [55338-70-0]
(2α,3β,4aβ,8aα)-*form*
Isol. as dihydrochloride.

Hydrochloride (1:2): [41627-96-7].
Mp 265-270°.

(2RS,3RS,4aSR,8aSR)-form [54933-08-3]
(2α,3β,4aα,8aβ)-*form*
Isol. as dihydrochloride.

Hydrochloride (1:2): [41597-42-6].
Mp 197-230° dec.

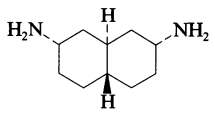
(2RS,3SR,4aSR,8aSR)-form [54933-09-4]
(2α,3α,4α,8β)-*form*
Isol. as dihydrochloride.

Hydrochloride (1:2): [41597-35-7].
Mp >254°.

Yano, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 985 (*synth, nmr*)

Decahydro-2,7-naphthalenediamine D-1-00007

2,7-Diaminodecalin. 2,7-Decalindiamine

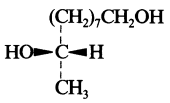


$C_{10}H_{20}N_2$ M 168.2

(2RS,4aRS,7SR,8aRS)-form
(2α,4aβ,7α,8aα)-*form*
Yellow needles (as picrate salt). Mp 243° (picrate).

Gross, R. *et al*, *Annalen*, 1994, 205.

1,9-Decanediol D-1-00008



(*S*)-*form*

$C_{10}H_{22}O_2$ M 174.2

(S)-form [128705-94-2]
Viscous oil; cryst. (Et_2O). Mp 28.5-30°. Bp_1 130°. $[\alpha]_D^{20}$ +7.5 (c, 1.614 in $CHCl_3$).

(±)-form [3208-05-7]
Cryst. (Et_2O). Mp 31.5-32.5°.

Quinkert, G. *et al*, *Helv. Chim. Acta*, 1989, **72**, 1753 (*synth, pmr, ir*)
Neeland, E.G. *et al*, *J.O.C.*, 1994, **59**, 7383 (*synth, pmr*)

2,4-Decanedione, 9CI D-1-00009

[13329-78-7]

$H_3CCOCH_2CO(CH_2)_5CH_3$

$C_{10}H_{18}O_2$ M 170.2
Oil. Bp_{17} 148-150°.

Yamauchi, M. *et al*, *Synthesis*, 1988, 178 (*synth, pmr*)
Ballini, R. *et al*, *Synthesis*, 1993, 965 (*synth, ir, pmr*)
Goosen, A. *et al*, *J.C.S. Perkin 2*, 1994, 557 (*synth, pmr, ms*)

4-Decenal D-1-00010

[30390-50-2]

$H_3C(CH_2)_4CH{=}CHCH_2CH_2CHO$

$C_{10}H_{18}O$ M 154.2

(E)-form [65405-70-1]

Used in perfumery. Pale yellow liq. with persistent green-aldehydic-floral odour. d 0.84. Bp_5 90°.

2,4-Dinitrophenylhydrazone: Mp 101-103°.

(Z)-form [21662-09-9]

Bp_{10} 78-80°.

Ger. Pat., 2 018 898, (1970); *CA*, **74**, 12612s.

Nikishin, G.I. *et al*, *Synthesis*, 1972, 376 (*synth, spectra*)

Bestmann, H.J. *et al*, *Annalen*, 1981, 1705 (*synth*)

6-Decenoic acid, 9CI D-1-00011

[85392-04-7]

$H_3CCH_2CH_2CH{=}CH(CH_2)_4COOH$

$C_{10}H_{18}O_2$ M 170.2

(E)-form

Liq. (?) with intense milky odour. Not yet found in nature (1986).

[86503-02-8, 86503-03-9, 86503-04-0, 118426-11-2]

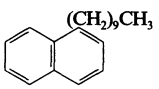
Tulloch, A.P. *et al*, *Chem. Phys. Lipids*, 1985, **37**, 197 (*cmr, Me ester*)

Shirakawa, T. *et al*, *Dev. Food Sci.*, 1988, **18**, 915 (*synth, occur*)

1-Decylnaphthalene D-1-00012

1-(1-Naphthalenyl)decane

[26438-27-7]



$C_{20}H_{28}$ M 268.4

d^{20} 0.932. Fp 15°. Bp 387°, Bp_1 168°. n_D^{20} 1.5435.

Adv. Chem. Ser., 1955, **15**, 232 (***props***)

2-Decylnaphthalene D-1-00013

1-(2-Naphthalenyl)decane

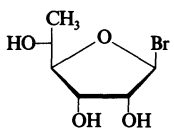
[14188-79-5]

$C_{20}H_{28}$ M 268.4

d^{20} 0.925. Fp 20°. Bp 387°, Bp_1 168°. n_D^{20} 1.5413.

Adv. Chem. Ser., 1955, **15**, 233 (***props***)

6-Deoxyallofuranosyl bromide D-1-00014



$C_6H_{11}BrO_4$ M 227.0

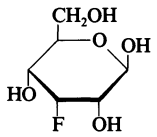
β-D-form

Tris(4-nitrobenzoyl): [80851-28-1].

Cryst. (CH_2Cl_2/hexane). Mp 118° (some dec. at 113°).

El-Khadem, H.S. *et al*, *Carbohydr. Res.*, 1981, **98**, 195 (*nitrobenzoyl, ir*)

3-Deoxy-3-fluoroallose D-1-00015



β-D-Pyranose-*form*

$C_6H_{11}FO_5$ M 182.1

β-D-Pyranose-form

Me glycoside: [87585-98-6].

$C_7H_{13}FO_5$ M 196.1 Solid. Mp 124-125°.

Me glycoside, 6-pivaloyl: [87586-03-6].

Cryst. (Et_2O). Mp 104.5-106°. $[\alpha]_D$ −48.8 (c, 1.0 in $CHCl_3$).

Me glycoside, 6-trityl: [87585-97-5].

Solid. Mp 84-86°.

Me glycoside, 4,6-O-isopropylidene: [87585-99-7].

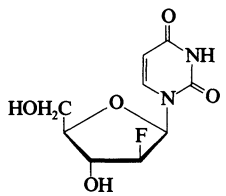
$C_{10}H_{17}FO_5$ M 236.2 Solid (Et_2O/hexane). Mp 84.5-87.5°.

Card, P.J. *et al*, *J.O.C.*, 1983, **48**, 4734 (*Me gly deriv, pmr, F-19 nmr*)

1-(2-Deoxy-2-fluoro-β-D-arabinofuranosyl)uracil D-1-00016

1-(2-Deoxy-2-fluoro-β-D-arabinofuranosyl)-2,4(1H,3H)-pyrimidinedione, 9CI

[69123-94-0]



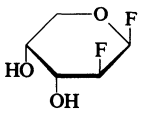
$C_9H_{11}FN_2O_5$ M 246.1

Cryst. (2-propanol/Et_2O). Mp 162° (156-157°).

Watanabe, K.A. *et al*, *J. Med. Chem.*, 1979, **22**, 21 (*synth*)

Sterzycki, R.Z. *et al*, *J. Med. Chem.*, 1990, **33**, 2150 (*synth, pmr, cmr*)

2-Deoxy-2-fluoroarabinopyranosyl fluoride D-1-00017



$C_5H_8F_2O_3$ M 154.1

β-D-form

Di-Ac: [30591-80-1].

$C_9H_{12}F_2O_5$ M 238.1 Cryst. (Et_2O/petrol). Mp 75-76°. $Bp_{0.5}$ 72-76° (bath). $[\alpha]_D^{22}$ −191.6 (c, 1.0 in $CHCl_3$), $[\alpha]_D^{23}$ −176 (c, 0.4 in $CHCl_3$).

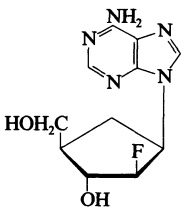
Dwek, R.A. *et al*, *Tet. Lett.*, 1970, 2987 (*synth*)

Albano, E.L. *et al*, *Carbohydr. Res.*, 1971, **19**, 63 (*di-Ac, pmr*)

Kent, P.W. *et al*, *Tetrahedron*, 1971, **27**, 3887 (*di-Ac, pmr, F-19 nmr*)

2′-Deoxy-2′-fluoro-*ara*-aristeromycin D-1-00018

Carbocyclic 2′-ara-fluoroadenosine



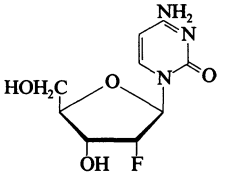
$C_{11}H_{14}FN_5O_2$ M 267.2

Powerful antiviral agent. Displays potent antiherpes activity *in vitro* and *in vivo*. Mp 109-113°. $[\alpha]_D^{22}$ +81 (H_2O).

Biggadike, K. *et al*, *Chem. Comm.*, 1988, 898 (*synth*)

2′-Deoxy-2′-fluorocytidine, 9CI D-1-00019

[10212-20-1]



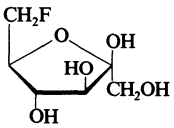
$C_9H_{12}FN_3O_4$ M 245.2

Needles (H_2O). Mp 171-173°. $[\alpha]_D^{26}$ +87 (c, 0.1 in H_2O).

Doerr, I.L. *et al*, *J.O.C.*, 1967, **32**, 1462 (*synth, uv*)

Kawasaki, A.M. *et al*, *J. Med. Chem.*, 1993, **36**, 831 (*synth, pmr, cmr*)

6-Deoxy-6-fluorofructose D-1-00020



$C_6H_{11}FO_5$ M 182.1

β-D-Furanose-form [99281-35-3]

Syrup.

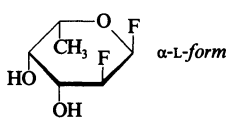
2,3-O-Isopropylidene, 1-tosyl: [83031-99-6].

Cryst. (MeOH). Mp 124-125°. $[\alpha]_D^{25}$ +15.5 ($CHCl_3$).

Guthrie, R.D. *et al*, *Aust. J. Chem.*, 1982, **35**, 1003 (*isopropyliene, pmr*)

Card, P.J. *et al*, *J.A.C.S.*, 1986, **108**, 158 (*β-D-fur*)

2-Deoxy-2-fluorofucopyranosyl fluoride D-1-00021



α-L-*form*

$C_6H_{10}F_2O_3$ M 168.1

α-L-form [84449-12-7]

Cryst. (Et_2O/petrol). Mp 120° dec. $[\alpha]_D^{22}$ −135 (c, 1.0 in MeOH).

Di-Ac: [74554-10-2].

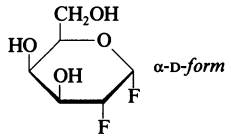
$C_{10}H_{14}F_2O_5$ M 252.2 Cryst. Mp 46.5-49° (46°). $[\alpha]_D^{22}$ −187.6 (−182) (c, 0.5 in $CHCl_3$).

β-L-form

Di-Ac: [84449-11-6].
Cryst. (Et_2O/petrol). Mp 85-86°. $[\alpha]_D^{22}$ −110 (c, 0.1 in $CHCl_3$).

Butchard, C.G. *et al, Tet. Lett.*, 1979, **35**, 2551 (*di-Ac*)
Korytnyk, W. *et al, Tetrahedron*, 1982, **38**, 2547 (*synth, pmr, F-19 nmr*)

2-Deoxy-2-fluorogalactopyranosyl fluoride D-1-00022



$C_6H_{10}F_2O_4$ M 184.1

α-D-form

$C_6H_{10}F_2O_4$ M 184.1
Cryst. (Et_2O, 2-propanol). Mp 163°. $[\alpha]_D^{22}$ +105 (c, 1.0 in MeOH).

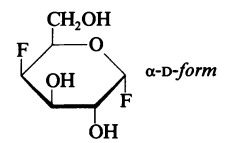
Tri-Ac: [28876-43-9].
$C_{12}H_{16}F_2O_7$ M 310.2 Cryst. (Et_2O/petrol). Mp 71-72° (68-70°). $[\alpha]_D$ +148.5 (c, 1.0 in $CHCl_3$).

β-D-form

Tri-Ac: [75414-44-7].
Needles (Et_2O/petrol). Mp 79.5-80°. $[\alpha]_D^{22}$ +84.5 (c, 1.0 in $CHCl_3$).

Adamson, J. *et al, Carbohydr. Res.*, 1970, **13**, 314; 1972, **22**, 257 (*tri-Ac, pmr*)
Dwek, R.A. *et al, Tet. Lett.*, 1970, 2987 (*tri-Ac, F-19 nmr*)
Korytnyk, W. *et al, Tetrahedron*, 1982, **38**, 2547 (*synth, pmr*)
Diksic, M. *et al, J. Carbohydr. Chem.*, 1985, **4**, 265 (*synth, F-19 nmr*)

4-Deoxy-4-fluorogalactopyranosyl fluoride D-1-00023



$C_6H_{10}F_2O_4$ M 184.1

α-D-form

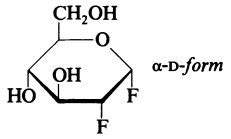
Tri-Ac: [40010-23-9].
$C_{12}H_{16}F_2O_7$ M 310.2 Cryst. (Et_2O/petrol). Mp 92-93°. $[\alpha]_D$ +112 (c, 1.0 in $CHCl_3$).

β-D-form

Tri-Ac: [40010-24-0].
Cryst. (Et_2O/petrol). Mp 88-89°. $[\alpha]_D$ +11 (c, 1.0 in $CHCl_3$).

Foster, A.B. *et al, Carbohydr. Res.*, 1972, **25**, 228 (*tri-Ac, pmr*)

2-Deoxy-2-fluoroglucopyranosyl fluoride D-1-00024



$C_6H_{10}F_2O_4$ M 184.1

α-D-form [75414-45-8]
Syrup. $[\alpha]_D^{20}$ +91.7 (c, 2.0 in MeOH).

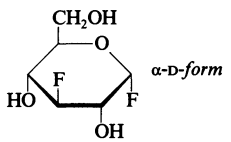
Tri-Ac: [24679-90-1].
$C_{12}H_{16}F_2O_7$ M 310.2 Cryst. (Et_2O/petrol). Mp 91-92° (69-70°). $[\alpha]_D^{20}$ +135 (c, 1.0 in $CHCl_3$).

β-D-form [103960-04-9]

Tri-Ac: [29069-93-0].
Cryst. (Et_2O/petrol). Mp 104-105° (99-101°). $[\alpha]_D^{20}$ +82 (c, 1.0 in $CDCl_3$) (+75).

Adamson, J. *et al, Carbohydr. Res.*, 1970, **15**, 351 (*α-tri-Ac, pmr*)
Hall, L.D. *et al, Can. J. Chem.*, 1971, **49**, 118 (*β-tri-Ac, F-19 nmr, pmr*)
Ido, T. *et al, J.O.C.*, 1977, **42**, 2341 (*α-tri-Ac, pmr*)
Korytnyk, W. *et al, Tetrahedron*, 1982, **38**, 2547 (*synth, α-form*)
Diksic, M. *et al, J. Carbohydr. Chem.*, 1985, **4**, 265 (*synth, F-19 nmr*)
Withers, S.G. *et al, J. Biol. Chem.*, 1988, **263**, 7929 (*F-19 nmr*)

3-Deoxy-3-fluoroglucopyranosyl fluoride D-1-00025



$C_6H_{10}F_2O_4$ M 184.1

α-D-form
Cryst. (MeCN). Mp 232° dec. $[\alpha]_D^{22}$ +99.8 (c, 2.0 in MeOH).

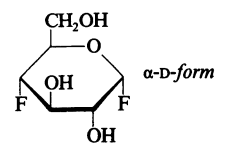
Tri-Ac: [31505-09-6].
$C_{12}H_{16}F_2O_7$ M 310.2 Syrup. $Bp_{0.1}$ 155-165° (bath). $[\alpha]_D^{23}$ +76 (c, 1.0 in $CHCl_3$).

β-D-form

Tri-Ac: [31505-10-9].
Cryst. (EtOH/petrol). Mp 79.5-80°. $[\alpha]_D^{25}$ +6 (c, 1.0 in $CHCl_3$).

Hall, L.D. *et al, Can. J. Chem.*, 1971, **49**, 236 (*tri-Ac, pmr, F-19 nmr*)
Klemm, G.H. *et al, Tet. Lett.*, 1982, 2927 (*tri-Ac, pmr*)

4-Deoxy-4-fluoroglucopyranosyl fluoride D-1-00026



$C_6H_{10}F_2O_4$ M 184.1

α-D-form

Tri-Ac: [33557-16-3].
$C_{12}H_{16}F_2O_7$ M 310.2 Syrup. $Bp_{0.15}$ 145-155° (bath). $[\alpha]_D$ +54 (c, 1.0 in $CHCl_3$).

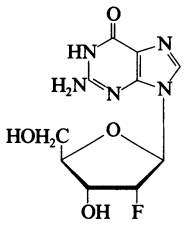
β-D-form

Tri-Ac: [33557-17-4].
Cryst. (Et_2O/petrol). $[\alpha]_D$ −26 (c, 1.0 in $CHCl_3$).

Barford, A.D. *et al, Carbohydr. Res.*, 1971, **19**, 49 (*tri-Ac, pmr, F-19 nmr*)

2′-Deoxy-2′-fluoroguanosine, 9CI D-1-00027

[78842-13-4]



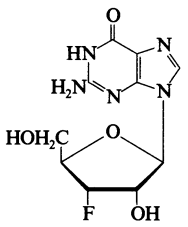
$C_{10}H_{12}FN_5O_4$ M 285.2
Needles (H_2O). Mp 240° dec.

Ikehara, M. *et al, Chem. Pharm. Bull.*, 1981, **29**, 3281 (*synth, uv, pmr, cmr*)
Kawasaki, A.M. *et al, J. Med. Chem.*, 1993, **36**, 831 (*synth, pmr, cmr*)

3′-Deoxy-3′-fluoroguanosine, 9CI D-1-00028

9-(3-Deoxy-3-fluoro-β-D-ribofuranosyl)guanine

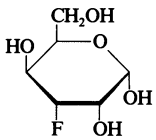
[123402-21-1]



$C_{10}H_{12}FN_5O_4$ M 285.2
Potent antiviral agent. Cryst. (H_2O). Mp 275-277°.

Puech, F. *et al, Chem. Comm.*, 1989, 955 (*synth, use*)

3-Deoxy-3-fluorogulose D-1-00029



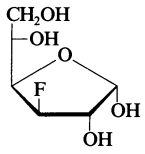
$C_6H_{11}FO_5$ M 182.1

α-D-Pyranose-form

Me glycoside: [32587-58-9]. *Methyl 3-deoxy-3-fluoro-α-D-gulopyranoside, 9CI*
$C_7H_{13}FO_5$ M 196.1 Cryst. Mp 123°. $[\alpha]_D^{28}$ +146 (c, 0.3 in MeOH).

Kent, P.W. *et al, Biochem. J.*, 1971, **121**, 10P (*Me gly*)
Kent, P.W. *et al, Tetrahedron*, 1971, **27**, 3887 (*Me gly, pmr, F-19 nmr*)

3-Deoxy-3-fluoroidose D-1-00030



β-L-Furanose-*form*

$C_6H_{11}FO_5$ M 182.1

L-form [35520-88-8]
Syrup. $[\alpha]_D$ −21 (H_2O).

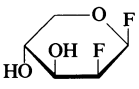
β-L-Furanose-form

1,2-O-Isopropylidene: [35520-87-7].
$C_9H_{15}FO_5$ M 222.2 Cryst. (Et_2O/hexane). Mp 105-106°.

1,2-O-Isopropylidene, 6-benzoyl: [35521-30-3].
$C_{16}H_{19}FO_6$ M 326.3 Cryst. (Et_2O/hexane). Mp 111-112°. $[\alpha]_D$ −8.5 (c, 1.0 in $CHCl_3$).

Brimacombe, J.S. *et al, Carbohydr. Res.*, 1972, **21**, 297 (*derivs, pmr, F-19 nmr*)

2-Deoxy-2-fluorolyxopyranosyl fluoride D-1-00031



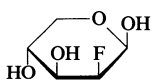
$C_5H_8F_2O_3$ M 154.1

β-D-form [34050-69-6]
Cryst. (EtOH/Et_2O). Mp 114°. $[\alpha]_D^{24}$ −142 (c, 0.22 in EtOH).

Di-Ac: [30591-78-7].
$C_9H_{12}F_2O_5$ M 238.1 Cryst. Mp 109-111°. $[\alpha]_D^{25}$ −114 (c, 0.5 in $CHCl_3$).

Butchard, C.G. *et al, Tetrahedron*, 1971, **27**, 3457 (*synth, pmr*)
Kent, P.W. *et al, Tetrahedron*, 1971, **27**, 3887 (*di-Ac, pmr, F-19 nmr*)

2-Deoxy-2-fluorolyxose D-1-00032



β-D-Pyranose-*form*

$C_5H_9FO_4$ M 152.1

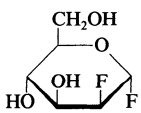
D-Pyranose-form [33983-50-5]
Cryst. (EtOH). Mp 124-126°. $[\alpha]_D^{24}$ −11.5 (c, 0.56 in H_2O).

β-D-Pyranose-form

Trifluoromethyl glycoside, di-Ac: [30591-79-8].
$C_{10}H_{12}F_4O_6$ M 304.1 Syrup. $[\alpha]_D^{24}$ −120 (c, 0.4 in $CHCl_3$).

Butchard, C.G. *et al, Tetrahedron*, 1971, **27**, 3457 (*synth, pmr, F-19 nmr*)
Kent, P.W. *et al, Tetrahedron*, 1971, **27**, 3887 (*deriv, pmr, F-19 nmr*)

2-Deoxy-2-fluoromannopyranosyl fluoride D-1-00033



α-D-*form*

$C_6H_{10}F_2O_4$ M 184.1

α-D-form

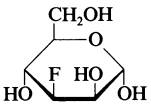
Tri-Ac: [29209-98-1].
$C_{12}H_{16}F_2O_7$ M 310.2 Cryst. (Et_2O/petrol). Mp 89-90°. $[\alpha]_D^{25}$ +27 ($CHCl_3$).

β-D-form

Tri-Ac: [24679-92-3].
Mp 114-115° (109-111°). $[\alpha]_D$ −2.5 ($CHCl_3$).

Hall, L.D. *et al, Can. J. Chem.*, 1971, **49**, 118 (*α-tri-Ac, pmr, F-19 nmr*)
Ido, T. *et al, J.O.C.*, 1977, **42**, 2341 (*β-tri-Ac, pmr*)
Korytnyk, W. *et al, Tetrahedron*, 1982, **38**, 2547 (*β-tri-Ac*)
Diksic, M. *et al, J. Carbohydr. Chem.*, 1985, **4**, 265 (*synth, F-19 nmr*)
Withers, S.G. *et al, Can. J. Chem.*, 1986, **64**, 232 (*synth, conformn, pmr, cryst struct*)

3-Deoxy-3-fluoromannose D-1-00034



α-D-Pyranose-*form*

$C_6H_{11}FO_5$ M 182.1

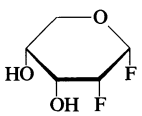
D-form [87764-46-3]
Needles (EtOH). Mp 173-175°. $[\alpha]_D$ +32 → +23 (c, 1.4 in H_2O).

Tetra-Ac: [88198-26-9].
$C_{14}H_{19}FO_9$ M 350.2 Cryst. Mp 116-117°. $[\alpha]_D$ +22 (c, 1.4 in $CHCl_3$).

[86258-31-3, 86334-54-5]

Rasmussen, J.R. *et al, Carbohydr. Res.*, 1983, **116**, 21 (*synth, cmr*)
Cerny, M. *et al, Coll. Czech. Chem. Comm.*, 1983, **48**, 2693 (*synth, tetra-Ac, pmr, F-19 nmr*)

2-Deoxy-2-fluororibopyranosyl fluoride D-1-00035



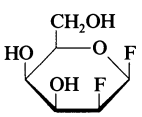
$C_5H_8F_2O_3$ M 154.1

α-D-form

Di-Ac: [33557-18-5].
$C_9H_{12}F_2O_5$ M 238.1 Cryst. Mp 87-88°. $[\alpha]_D^{22}$ +82.8 (c, 0.9 in $CHCl_3$).

Albano, E.L. *et al, Carbohydr. Res.*, 1971, **19**, 63 (*di-Ac, pmr, F-19 nmr*)

2-Deoxy-2-fluorotalopyranosyl fluoride D-1-00036



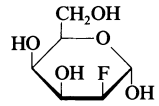
$C_6H_{10}F_2O_4$ M 184.1

β-D-form

Tri-Ac: [35526-13-7].
$C_{12}H_{16}F_2O_7$ M 310.2 Syrup. $Bp_{0.17}$ 168-170°. $[\alpha]_D$ +19 ($CHCl_3$).

Adamson, J. *et al, Carbohydr. Res.*, 1972, **22**, 257 (*tri-Ac*)
Korytnyk, W. *et al, Tetrahedron*, 1982, **38**, 2547 (*tri-Ac, pmr*)

2-Deoxy-2-fluorotalose D-1-00037



α-D-Pyranose-*form*

$C_6H_{11}FO_5$ M 182.1

α-D-Pyranose-form [98856-45-2]
Syrup.

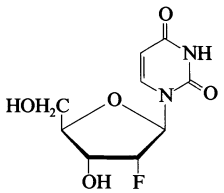
β-D-Pyranose-form [98856-46-3]
Syrup.

Trifluoromethyl glycoside, tri-Ac: [35526-12-6].
$C_{13}H_{16}F_4O_8$ M 376.2 $Bp_{0.15}$ 148-150°. $[\alpha]_D$ +1.9 (c, 3.0 in $CHCl_3$).

Adamson, J. *et al, Carbohydr. Res.*, 1972, **22**, 257 (*deriv, pmr, F-19 nmr*)
Diksic, M. *et al, J. Carbohydr. Chem.*, 1985, **4**, 265 (*synth, F-19 nmr*)

2′-Deoxy-2′-fluorouridine, 9CI D-1-00038

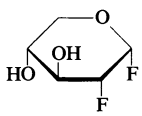
[784-71-4]



$C_9H_{11}FN_2O_5$ M 246.1
Cryst. (EtOH). Mp 150-151°. $[\alpha]_D^{20}$ +52 (c, 0.3 in H_2O).

Codington, J.F. *et al, J.O.C.*, 1964, **29**, 558 (*synth*)
Kawasaki, A.M. *et al, J. Med. Chem.*, 1993, **36**, 361 (*synth, pmr, cmr*)

2-Deoxy-2-fluoroxylopyranosyl fluoride D-1-00039



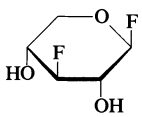
$C_5H_8F_2O_3$ M 154.1

α-D-form

Di-Ac: [30591-82-3].
$C_9H_{12}F_2O_5$ M 238.1 Syrup.

Dwek, R.A. *et al, Tet. Lett.*, 1970, 2987 (*di-Ac, F-19 nmr*)
Kent, P.W. *et al, Tetrahedron*, 1971, **27**, 3887 (*di-Ac, config, F-19 nmr*)

3-Deoxy-3-fluoroxylopyranosyl fluoride D-1-00040



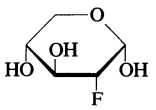
$C_5H_8F_2O_3$ M 154.1

β-D-form

Di-Ac: [31505-11-0].
$C_9H_{12}F_2O_5$ M 238.1 Cryst. ($CHCl_3$/petrol). Mp 58°. $[\alpha]_D^{20}$ −67 (c, 1.0 in $CHCl_3$).

Hall, L.D. *et al, Can. J. Chem.*, 1971, **49**, 236 (*di-Ac, F-19 nmr, pmr*)

2-Deoxy-2-fluoroxylose D-1-00041


α-D-Pyranose-*form*

$C_5H_9FO_4$ M 152.1

D-form [28867-50-7]
Syrup. $[\alpha]_D^{23}$ +69 (15 min.) → +32 (1h) (c, 0.9 in EtOH).

α-D-Pyranose-form [129939-84-0]

Trifluoromethyl glycoside, di-Ac: [30591-83-4].
$C_{10}H_{12}F_4O_6$ M 304.1 Cryst. (Et_2O/petrol). Mp 150°. $[\alpha]_D^{24}$ +130 (c, 0.37 in $CHCl_3$).

β-D-Pyranose-form [129939-83-9]
Syrup.

β-D-Furanose-form

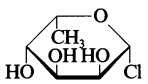
Me glycoside: [28867-49-4].
$C_6H_{11}FO_4$ M 166.1 Oil. $[\alpha]_D^{23}$ −102 (c, 1.4 in EtOH).

Me glycoside, 3-benzoyl, 5-benzyl: [28867-51-8].
$C_{20}H_{21}FO_5$ M 360.3 Syrup. $[\alpha]_D^{23}$ −63 (c, 1.2 in EtOH).

Me glycoside, 5-benzyl: [28867-48-3].
$C_{13}H_{17}FO_4$ M 256.2 Pale yellow syrup. $[\alpha]_D^{23}$ −42 (c, 0.9 in EtOH).

Wright, J.A. *et al, Carbohydr. Res.*, 1970, **13**, 297 (D-form, β-Me fur, β-Me fur derivs, pmr)
Kent, P.W. *et al, Tetrahedron*, 1971, **27**, 3457, 3887 (α-D-pyr deriv, pmr, F-19 nmr)
Bols, M. *et al, Acta Chem. Scand.*, 1990, **44**, 252 (*synth, pmr*)

6-Deoxygulopyranosyl chloride D-1-00042



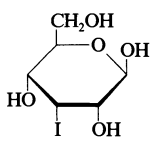
$C_6H_{11}ClO_4$ M 182.6

β-L-form

2,3-O-Isopropylidene, 4-Me: [65904-40-7].
$C_{10}H_{17}ClO_4$ M 236.6 Oil. $Bp_{0.015}$ 65°. $[\alpha]_D^{23}$ +45.3 (c, 1.23 in $CHCl_3$).

Ireland, R.E. *et al, J.O.C.*, 1978, **43**, 786; 1980, **45**, 48 (*isopropylidene deriv, pmr*)

3-Deoxy-3-iodoallose D-1-00043


β-D-Pyranose-*form*

$C_6H_{11}IO_5$ M 290.0

β-D-Pyranose-form

Me glycoside, 4,6-O-benzylidene: [117605-32-0].
$C_{14}H_{17}IO_5$ M 392.1 Cryst. Mp 151-152°. $[\alpha]_D^{22}$ +1.62 (c, 2.22 in $CHCl_3$).

Me glycoside, 4,6-O-(4-methoxybenzylidene): [117605-33-1].
Syrup. $[\alpha]_D^{22}$ −27 (c, 0.89 in $CHCl_3$).

α-D-Furanose-form

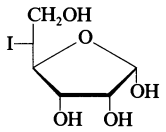
1,2-O-Isopropylidene: [114192-72-2].
$C_9H_{15}IO_5$ M 330.1 Oil.

1,2-O-Isopropylidene, 5,6-dimesyl: [114192-73-3].
$C_{11}H_{19}IO_9S_2$ M 486.3 Cryst. (EtOAc/petrol). Mp 146°. $[\alpha]_D$ +69 (c, 0.7 in $CHCl_3$).

1,2:5,6-Di-O-isopropylidene: [67337-61-5].
$C_{12}H_{19}IO_5$ M 370.1 Mp 55-56°. $[\alpha]_D^{22}$ +64 (c, 2.0 in $CHCl_3$), $[\alpha]_D$ +79.5 (c, 0.6 in C_6H_6).

Kunz, H. *et al, Annalen*, 1982, 1245 (*diisopropylidene*)
Gurjar, M.K. *et al, Carbohydr. Res.*, 1987, **165**, 313 (*dimesyl*)
Classon, B. *et al, J.O.C.*, 1988, **53**, 6126 (*β-Me gly deriv, pmr, cmr*)
Russell, R.N. *et al, Carbohydr. Res.*, 1990, **201**, 95 (*diisopropylidene, pmr, cmr*)
Marco-Contelles, J.L. *et al, Synlett*, 1990, 167 (*isopropylidene*)

5-Deoxy-5-iodoallose D-1-00044



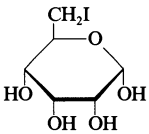
$C_6H_{11}IO_5$ M 290.0

α-D-Furanose-form

1,2-O-Isopropylidene, 3,6-dibenzoyl: [55085-26-2].
$C_{23}H_{23}IO_7$ M 538.3 Cryst. (EtOH). Mp 65-67°. $[\alpha]_D^{20}$ +60 (c, 0.3 in CH_2Cl_2).

Serge, D. *et al, C. R. Hebd. Seances Acad. Sci. Ser. C*, 1974, **279**, 651 (*isopropylidene deriv*)
Serge, D. *et al, Carbohydr. Res.*, 1979, **77**, 79 (*isopropylidene deriv*)

6-Deoxy-6-iodoallose D-1-00045


α-D-Pyranose-*form*

$C_6H_{11}IO_5$ M 290.0

α-D-Pyranose-form

Me glycoside: [56571-02-9]. *Methyl 6-deoxy-6-iodo-α-D-allopyranoside*
$C_7H_{13}IO_5$ M 304.0 Cryst. (EtOAc/hexane). Mp 81°. $[\alpha]_D^{22}$ +85.3 (c, 1.75 in $CHCl_3$).

Me glycoside, tri-Ac: [56570-98-0].
$C_{13}H_{19}IO_8$ M 430.1 Cryst. (Et_2O/hexane). Mp 75°. $[\alpha]_D^{22}$ +72.2 (c, 1.4 in $CHCl_3$).

Me glycoside, 2,3-dibenzoyl, 4-Ac: [109681-64-3].
$C_{23}H_{23}IO_8$ M 554.3 Amorph. powder. $[\alpha]_D^{22}$ +46.3 (c, 1.31 in $CHCl_3$).

Me glycoside, 3-(tetrahydropyran-2-yl), 2-Ac: [107599-43-9].
Oil. $[\alpha]_D^{20}$ +34.7 (c, 3.0 in $CHCl_3$).

β-D-Pyranose-form

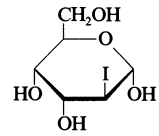
Me glycoside: [56571-03-0]. *Methyl 6-deoxy-6-iodo-β-D-allopyranoside*
$C_7H_{13}IO_5$ M 304.0 Cryst. (EtOAc/MeOH). Mp 72°. $[\alpha]_D^{22}$ −38.8 (c, 2.0 in CH_3OH).

Me glycoside, tri-Ac: [56570-99-1].
Cryst. (hexane). Mp 85°. $[\alpha]_D^{22}$ −33.8 (c, 1.0 in $CHCl_3$).

[114925-88-1, 114925-89-2]

Lehmann, J. *et al, Carbohydr. Res.*, 1975, **42**, 275 (*α-Me gly, β-Me gly, tri-Ac*)
Mori, M. *et al, Chem. Pharm. Bull.*, 1986, **34**, 4037 (*4-Ac deriv, ir, pmr*)
Nicolaou, K.C. *et al, J.A.C.S.*, 1987, **109**, 2821; 1988, **110**, 4696 (*tetrahydropyranyl, ir, pmr*)

2-Deoxy-2-iodoaltrose D-1-00046


α-D-Pyranose-*form*

$C_6H_{11}IO_5$ M 290.0

α-D-Pyranose-form

Me glycoside: [71019-18-6].
$C_7H_{13}IO_5$ M 304.0 Needles (Me_2CO). Mp 134° dec. $[\alpha]_D^{22}$ +44 (c, 1.0 in H_2O). Unstable to heat and light.

Me glycoside, tri-Ac: [106023-34-1].
$C_{13}H_{19}IO_8$ M 430.1 Oil. $[\alpha]_D^{20}$ +21.7 (c, 2.0 in $CHCl_3$).

Me glycoside, 3,4-O-benzylidene (R-)*:* [35775-00-9].
$C_{14}H_{17}IO_5$ M 392.1 Syrup.

Me glycoside, 3,4-O-benzylidene (S-)*:* [35775-04-3].
$C_{14}H_{17}IO_5$ M 392.1 Cryst. (petrol). Mp 100°. $[\alpha]_D^{20}$ +35 (c, 1.0 in $CHCl_3$).

Me glycoside, 4,6-O-benzylidene: [14125-73-6].
$C_{14}H_{17}IO_5$ M 392.1 Cryst. (Et_2O/hexane or EtOH). Mp 105-106°. $[\alpha]_D^{20}$ +41 (c, 1.5 in $CHCl_3$), $[\alpha]_D^{25}$ +35 (c, 2.0 in $CHCl_3$).

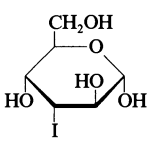
β-D-Pyranose-form

Me glycoside, 4,6-O-benzylidene: [18968-73-5].
Cryst. (EtOH). Mp 175-176°. $[\alpha]_D^{25}$ −91 (c, 2.8 in $CHCl_3$).

Me glycoside, 4,6-O-benzylidene, 3-Ac: [18968-74-6].
$C_{16}H_{19}IO_6$ M 434.2 Needles. Mp 123-123.5°. $[\alpha]_D^{25}$ −109 (c, 3.0 in $CHCl_3$).

Lemieux, R.U. *et al, Can. J. Chem.*, 1968, **46**, 61 (*α-Me gly deriv, β-Me gly deriv*)
Inch, T.D. *et al, Carbohydr. Res.*, 1972, **21**, 37 (*3,4-benzylidene*)
Guthrie, R.D. *et al, Carbohydr. Res.*, 1979, **72**, 285 (*α-Me gly*)
Furstner, A. *et al, J.O.C.*, 1989, **54**, 2307 (*4,6-benzylidene, pmr*)

3-Deoxy-3-iodoaltrose D-1-00047



$C_6H_{11}IO_5$ M 290.0

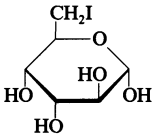
α-D-Pyranose-form

Me glycoside, 4,6-O-benzylidene: [56981-10-3].
$C_{14}H_{17}IO_5$ M 392.1 Rods (EtOAc). Mp 163.5-164.5°. $[\alpha]_D^{23}$ +117 (+111) (c, 4.0 in $CHCl_3$).

Me glycoside, 4,6-O-benzylidene, 2-tosyl: Cryst. (EtOH). Mp 128-129°. $[\alpha]_D^{23}$ +46.4 ($CHCl_3$) (+37.5). Unstable at r.t., dec. to a dark tar.

Richards, G.N. *et al, J.C.S.*, 1954, 4511; 1956, 496 (*benzylidene*)
Lemieux, R.U. *et al, Can. J. Chem.*, 1968, **46**, 61 (*2-tosyl*)
Hicks, D.R. *et al, Can. J. Chem.*, 1975, **53**, 2017 (*benzylidene*)

6-Deoxy-6-iodoaltrose D-1-00048



$C_6H_{11}IO_5$ M 290.0

α-D-Pyranose-form

Me glycoside: $C_7H_{13}IO_5$ M 304.0 Cryst. Mp 105-106°. $[\alpha]_D$ +91.4 ($CHCl_3$).

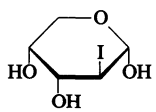
Me glycoside, tribenzoyl: $C_{28}H_{25}IO_8$ M 616.4 Cryst. Mp 143-145°. $[\alpha]_D$ +2.5 ($CHCl_3$).

Me glycoside, 2,3-dibenzyl: [118068-39-6]. $C_{21}H_{25}IO_5$ M 484.3 Syrup. $[\alpha]_D^{27}$ +51 (c, 1.0 in $CHCl_3$).

Me glycoside, 2,3-dibenzyl, 4-Ac: [127213-05-2]. $C_{23}H_{27}IO_6$ M 526.3 Syrup. $[\alpha]_D^{27}$ +21 (c, 0.25 in $CHCl_3$).

Rosenfeld, D.A. *et al, J.A.C.S.*, 1948, **70**, 2204 (*Me gly*)
Noritaka, C. *et al, Bull. Chem. Soc. Jpn.*, 1991, **64**, 2118 (*4-Ac, pmr, ir*)
Chida, N. *et al, J.O.C.*, 1991, **56**, 2976 (*dibenzyl, ir, pmr*)

2-Deoxy-2-iodoarabinose D-1-00049



α-D-Pyranose-*form*

$C_5H_9IO_4$ M 260.0

α-D-Pyranose-form

Me glycoside, 3,4-di-Ac: [131337-13-8]. $C_{10}H_{15}IO_6$ M 358.1 Cryst. (Et_2O/hexane). Mp 100-101°. $[\alpha]_D^{20}$ −51.2 (c, 1.0 in $CHCl_3$).

α-L-Pyranose-form

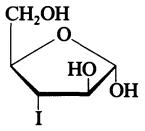
Me glycoside, 3,4-di-Ac: [26528-48-3]. $C_{10}H_{15}IO_6$ M 358.1 Cryst. (Et_2O/petrol). Mp 100-101.5°.

β-L-Pyranose-form

Me glycoside, 4-benzoyl: [26528-17-6]. $C_{13}H_{15}IO_5$ M 378.1 Cryst. (EtOH). Mp 96-97°. $[\alpha]_D^{25}$ +144 (c, 2.32 in $CHCl_3$).

Lemieux, R.U. *et al, Can. J. Chem.*, 1969, **47**, 4413, 4427 (α-L-Me gly deriv, β-L-Me gly deriv, pmr)
Horton, D. *et al, Carbohydr. Res.*, 1990, **205**, 71 (α-D-Me gly deriv, pmr)

3-Deoxy-3-iodoarabinose D-1-00050



$C_5H_9IO_4$ M 260.0

α-D-Furanose-form

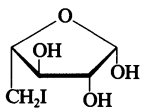
Me glycoside, 5-benzoyl: [26532-12-7]. $C_{13}H_{15}IO_5$ M 378.1 Syrup. $[\alpha]_D^{25}$ +73.1 (c, 1.58 in $CHCl_3$).

Me glycoside, 5-(4-nitrobenzoyl): [53081-37-1]. Pale yellow needles (Et_2O/petrol). Mp 101-102°. $[\alpha]_D^{22}$ +79.5 (c, 1.0 in $CHCl_3$).

Me glycoside, 2,5-bis-(4-nitrobenzoyl): [53081-38-2]. Pale yellow needles (CH_2Cl_2/hexane). Mp 185°. $[\alpha]_D^{22}$ −1.09 (c, 1.0 in CH_2Cl_2).

Lemieux, R.U. *et al, Can. J. Chem.*, 1969, **47**, 4413 (*benzoyl*)
El Khadem, H.S. *et al, Carbohydr. Res.*, 1974, **33**, 329 (*nitrobenzoyl, ir, pmr*)

5-Deoxy-5-iodoarabinose D-1-00051



β-L-Furanose-*form*

$C_5H_9IO_4$ M 260.0

L-form

Ethylene dithioacetal, 2,3,4-tri-Ac: [17073-62-0]. $C_{13}H_{19}IO_6S_2$ M 462.3 Cryst. (EtOH). Mp 110-110.5°.

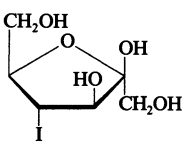
β-L-Furanose-form

1,2-O-Isopropylidene: [84936-06-1]. $C_8H_{13}IO_4$ M 300.0 Needles (EtOAc/petrol). Mp 66-67°. $[\alpha]_D^{27}$ +6.86 ($CHCl_3$).

1,2-O-Isopropylidene, 3-Ac: [20853-30-9]. $C_{10}H_{15}IO_5$ M 342.1 Syrup.

Levene, P.A. *et al, J. Biol. Chem.*, 1936, **116**, 189 (*β*-L-fur deriv)
Fernandez-Bolanos, J. *et al, An. R. Soc. Esp. Fis. Quim., Ser. B*, 1966, **62**, 1069; *CA*, **67**, 82339n (*dithioacetal*)
Hough, L. *et al, Adv. Chem. Ser.*, 1968, 120; *CA*, **69**, 97035a (*β*-L-fur deriv)
Binkley, R.W. *et al, J. Carbohydr. Chem.*, 1982, **1**, 213 (*β*-L-fur deriv)

4-Deoxy-4-iodofructose D-1-00052



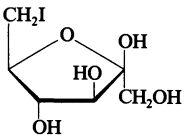
$C_6H_{11}IO_5$ M 290.0

β-D-Furanose-form

Me glycoside, tri-Ac: [82078-04-4]. $C_{13}H_{19}IO_8$ M 430.1 Syrup. $[\alpha]_D$ −52 (c, 1.0 in $CHCl_3$).

Guthrie, R.D. *et al, Carbohydr. Res.*, 1982, **103**, 1 (*tri-Ac, cmr*)

6-Deoxy-6-iodofructose D-1-00053



β-D-Furanose-*form*

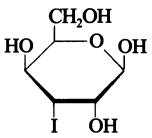
$C_6H_{11}IO_5$ M 290.0

β-D-Furanose-form

2,3-O-Isopropylidene, 1-tosyl: [83032-12-6]. Cryst. ($CHCl_3$/hexane). Mp 124-125°. $[\alpha]_D^{25}$ +5.6 ($CHCl_3$), $[\alpha]_D$ +7.5 (c, 3.2 in MeOH).

Morgan, W.T.J. *et al, Helv. Chim. Acta*, 1938, **21**, 1023 (*deriv*)
Guthrie, R.D. *et al, Aust. J. Chem.*, 1982, **35**, 1003 (*deriv, pmr*)

3-Deoxy-3-iodogulose D-1-00054



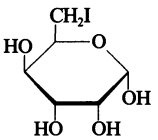
$C_6H_{11}IO_5$ M 290.0

β-D-Pyranose-form

Me glycoside, tribenzoyl: [124314-31-4]. $C_{28}H_{25}IO_8$ M 616.4 Glass. $[\alpha]_D^{25}$ +61 (c, 0.6 in $CHCl_3$).

Lin, T.-H. *et al, Carbohydr. Res.*, 1989, **188**, 228 (*tribenzoyl, cmr*)

6-Deoxy-6-iodogulose D-1-00055



$C_6H_{11}IO_5$ M 290.0

α-D-Pyranose-form

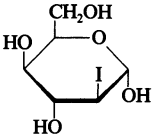
Me glycoside, 3-benzyl, 2-tosyl: [96691-86-0]. $C_{21}H_{25}IO_7S$ M 548.3 Syrup. $[\alpha]_D$ +143 (c, 1.0 in $CHCl_3$).

Me glycoside, 3-benzyl, 4-benzoyl, 2-tosyl: [96691-87-1]. $C_{28}H_{29}IO_8S$ M 652.5 Syrup. $[\alpha]_D$ +54 (c, 1.0 in $CHCl_3$).

Me glycoside, 3,4-dibenzyl, 2-tosyl: [96691-88-2]. $C_{28}H_{31}IO_7S$ M 638.5 Syrup. $[\alpha]_D$ +25 ($CHCl_3$).

Ferrier, R.J. *et al, J.C.S. Perkin 1*, 1985, 301 (*Me gly deriv, pmr*)

2-Deoxy-2-iodoidose D-1-00056



$C_6H_{11}IO_5$ M 290.0

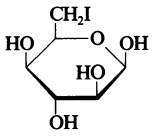
α-D-Pyranose-form

Me glycoside, 4,6-O-benzylidene: [18968-77-9]. $C_{14}H_{17}IO_5$ M 392.1 Needles (EtOH). Mp 162-163°. $[\alpha]_D^{25}$ +28 (c, 1.2 in $CHCl_3$).

Me glycoside, 4,6-O-benzylidene, 3-Ac: [18968-82-6].
$C_{16}H_{19}IO_6$ M 434.2 Cubes. Mp 174-175°. $[\alpha]_D^{25}$ −28 (c, 2.4 in $CHCl_3$).

Lemieux, R.U. *et al, Can. J. Chem.*, 1968, **46**, 61 (*Me gly derivs*)

6-Deoxy-6-iodoidose D-1-00057



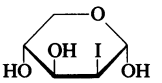
$C_6H_{11}IO_5$ M 290.0

β-D-Pyranose-form

Me glycoside, 3-Me, 2,4-ditosyl:
$C_{22}H_{27}IO_9S_2$ M 626.4 Syrup.

Fischer, R. *et al, Helv. Chim. Acta*, 1954, **37**, 6 (*Me gly deriv*)

2-Deoxy-2-iodolyxose D-1-00058



α-D-Pyranose-*form*

$C_5H_9IO_4$ M 260.0

α-D-Pyranose-form

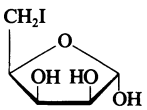
Me glycoside, di-Ac: [51385-07-0].
$C_{10}H_{15}IO_6$ M 358.1 Cryst. Mp 116°. $[\alpha]_D^{25}$ −17 (c, 1.65 in $CHCl_3$). Dec. when stored at r.t.

α-L-Pyranose-form

Me glycoside, di-Ac: [131267-50-0].
Cryst. (Et_2O/hexane). Mp 115-117°. $[\alpha]_D^{20}$ +14.9 (c, 1.0 in $CHCl_3$).

Van Es, T., *J. S. Afr. Chem. Inst.*, 1973, **26**, 152 (D-Me gly deriv, pmr)
Horton, D. *et al, Carbohydr. Res.*, 1990, **205**, 71 (L-Me gly deriv, pmr)

5-Deoxy-5-iodolyxose D-1-00059



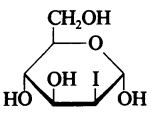
$C_5H_9IO_4$ M 260.0

α-D-Furanose-form

Me glycoside, 2,3-O-isopropylidene: [63087-96-7].
$C_9H_{15}IO_4$ M 314.1 Oil. $[\alpha]_D^{20}$ +75.4 (c, 9.0 in CH_2Cl_2), $[\alpha]_D^{24}$ +72.6 (c, 2.88 in MeOH).

Fuersther, A. *et al, J.O.C.*, 1991, **56**, 2213 (*Me gly deriv, pmr*)

2-Deoxy-2-iodomannose D-1-00060



α-D-Pyranose-*form*

$C_6H_{11}IO_5$ M 290.0

D-form

Syrup.

α-D-Pyranose-form

3,4,6-Tri-Ac: [53008-86-9].
$C_{12}H_{17}IO_8$ M 416.1 Syrup. $[\alpha]_D^{35}$ −18.8 (c, 1.4 in $CHCl_3$).

1-Benzoyl, 3,4,6-tri-Ac: [20846-99-5].
$C_{19}H_{21}IO_9$ M 520.2 Cryst. Mp 160-161°. $[\alpha]_D$ +45.3 (c, 2.0 in $CHCl_3$).

Me glycoside: [10226-88-7]. *Methyl 2-deoxy-2-iodo-α-D-mannopyranoside*
$C_7H_{13}IO_5$ M 304.0 Cryst. Mp 145-146°. $[\alpha]_D$ +49.2 (c, 1.0 in MeOH).

Me glycoside, tri-Ac: [20701-50-2].
$C_{13}H_{19}IO_8$ M 430.1 Syrup. $[\alpha]_D$ +44.9 ($CHCl_3$).

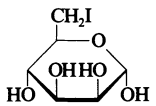
β-D-Pyranose-form

Me glycoside: [53008-76-7]. *Methyl 2-deoxy-2-iodo-β-D-mannopyranoside*
$C_7H_{13}IO_5$ M 304.0 Needles ($MeOH/Et_2O$). Mp 147-148°. $[\alpha]_D^{28}$ −6.3 (c, 0.7 in MeOH).

Me glycoside, tri-Ac: [53008-74-5].
Cryst. (Et_2O/hexane). Mp 118-118.5°. $[\alpha]_D^{27}$ −97.8 (c, 1.9 in $CHCl_3$).

Lemieux, R.U. *et al, Can. J. Chem.*, 1962, **40**, 1926 (*α-Me gly*)
Hall, L.D. *et al, Can. J. Chem.*, 1969, **47**, 361 (*1-benzoyl*)
Honda, S. *et al, Carbohydr. Res.*, 1974, **34**, 45 (D-form, α-tri-Ac, α-Me gly, β-Me gly)
Horton, D. *et al, Carbohydr. Res.*, 1990, **205**, 71 (*α-tri-Ac*)

6-Deoxy-6-iodomannose D-1-00061



α-D-Pyranose-*form*

$C_6H_{11}IO_5$ M 290.0

α-D-Pyranose-form

Me glycoside: [52290-43-4]. *Methyl 6-deoxy-6-iodo-α-D-mannopyranoside*
$C_7H_{13}IO_5$ M 304.0 Cryst. Mp 120-122°. $[\alpha]_D$ +55 (H_2O).

Me glycoside, tri-Ac: [50692-55-2].
$C_{13}H_{19}IO_8$ M 430.1 Cryst. (EtOH). Mp 91-92°. $[\alpha]_D^{22}$ +48 (c, 1.2 in $CHCl_3$).

Me glycoside, 2,3-dimesyl: [118360-72-8].
$C_9H_{17}IO_9S_2$ M 460.2 Amorph. solid. $[\alpha]_D^{31}$ +29 (c, 0.6 in $CHCl_3$).

Me glycoside, 2,3-O-isopropylidene: [22932-34-9].
$C_{10}H_{17}IO_5$ M 344.1 Cryst. Mp 111-112° (109-110°). $[\alpha]_D^{24}$ +44.2 (c, 1.0 in MeOH), $[\alpha]_D^{20}$ +46 (c, 1.3 in $CHCl_3$).

Me glycoside, 2,3-O-isopropylidene, 4-benzoyl: [122805-35-0].
$C_{17}H_{21}IO_6$ M 448.2 Cryst. (EtOH). Mp 159-161°. $[\alpha]_D^{22}$ +10.5 (c, 1.85 in $CHCl_3$).

Me glycoside, 2,3-O-isopropylidene, 4-mesyl: [22932-31-6].
$C_{11}H_{19}IO_7S$ M 422.2 Cryst. Mp 84.5-85°. $Subl._{0.0005}$ 80° (bath). $[\alpha]_D^{28}$ +23.9 (c, 1.03 in $CHCl_3$).

Me glycoside, 2,3-O-isopropylidene, 4-brosyl: [22932-33-8].
$C_{16}H_{20}BrIO_7S$ M 563.2 Needles ($EtOH/Et_2O$). Mp 86-87.5°. $[\alpha]_D^{24}$ +2.4 (c, 1.0 in MeOH).

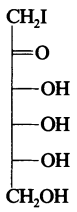
β-D-Pyranose-form

Me glycoside: [56571-01-8]. *Methyl 6-deoxy-6-iodo-β-D-mannopyranoside*
$C_7H_{13}IO_5$ M 304.0 Cryst. (EtOAc). Mp 127°. $[\alpha]_D^{22}$ −26.2 (c, 1.9 in MeOH).

Me glycoside, tri-Ac: [56570-97-9].
Cryst. (Et_2O/hexane). Mp 120°. $[\alpha]_D^{22}$ −16 (c, 1.0 in $CHCl_3$).

Lehmann, J. *et al, J.A.C.S.*, 1964, **86**, 4496 (*α-Me pyr*)
Stevens, C.L. *et al, J.O.C.*, 1970, **35**, 592 (*isopropylidene, 4-mesyl, 4-brosyl*)
Lehmann, J. *et al, Carbohydr. Res.*, 1975, **42**, 275 (*β-Me pyr deriv*)
Tatsuta, K. *et al, Bull. Chem. Soc. Jpn.*, 1988, **61**, 2525 (*dimesyl*)
Bundle, D.R. *et al, Carbohydr. Res.*, 1988, **174**, 239 (*isopropylidene, pmr*)
Classon, B. *et al, J.O.C.*, 1988, **53**, 6126 (*tri-Ac*)
Tsvetkov, Y.E. *et al, Bioorg. Khim.*, 1989, **15**, 231; *Sov. J. Bioorg. Chem. (Engl. Transl.)*, 1989, **15**, 126 (*4-benzoyl, pmr*)

1-Deoxy-1-iodopsicose D-1-00062



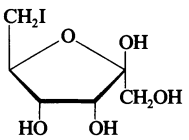
$C_6H_{11}IO_5$ M 290.0

D-form

Tetra-Ac:
$C_{14}H_{19}IO_9$ M 458.2 Cryst. Mp 64-65°. $[\alpha]_D$ +6.8 ($CHCl_3$).

Wolfrom, M.L. *et al, J.A.C.S.*, 1945, **67**, 1793 (*tetra-Ac*)
Vanek, T. *et al, Coll. Czech. Chem. Comm.*, 1979, **44**, 1339 (*tetra-Ac*)

6-Deoxy-6-iodopsicose D-1-00063



β-D-Furanose-*form*

$C_6H_{11}IO_5$ M 290.0

D-Furanose-form [58463-06-2]
Cryst. ($Me_2CO/CHCl_3$). Mp 80.5-81°. $[\alpha]_D^{23}$ +14.6 (c, 1 in H_2O).

Tetrabenzoyl: [58463-07-3].
$C_{34}H_{27}IO_9$ M 706.4 Foam.

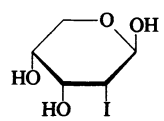
Tetrakis(p-*nitrobenzoyl*): [58463-08-4].
Cryst. ($CHCl_3$/hexane). Mp 173-174°.

β-D-Furanose-form

1,2:3,4-Di-O-isopropylidene: [38084-06-9].
$C_{12}H_{19}IO_5$ M 370.1 Cryst. (MeOH aq. or hexane). Mp 46-47° (44-44.5°). $[\alpha]_D^{23}$ −74.3 (c, 0.5 in $CHCl_3$).

James, K. *et al, Aust. J. Chem.*, 1972, **25**, 1967 (*diisopropylidene, pmr*)
Prisbe, E.J. *et al, J.O.C.*, 1976, **41**, 1836 (*synth, deriv, pmr, cmr*)

2-Deoxy-2-iodoribose D-1-00064



β-D-Pyranose-*form*

$C_5H_9IO_4$ M 260.0

β-D-Pyranose-form

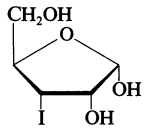
Me glycoside, 3,4-di-Ac: [131267-52-2].
$C_{10}H_{15}IO_6$ M 358.1 Syrup. $Bp_{0.04}$ 90°. $[\alpha]_D^{20}$ +10.7 (c, 1 in $CHCl_3$).

Me glycoside, 1-benzoyl, 3,4-di-Ac: [22854-36-0].
$C_{16}H_{17}IO_7$ M 448.2 Cryst. Mp 129-130° (EtOH aq.). $[\alpha]_D^{27}$ −26.5 (c, 1.46 in $CHCl_3$).

β-D-Furanose-form [125155-50-2]
Syrup.

Hall, L.D. *et al, Can. J. Chem.*, 1969, **47**, 361 (*β-pyr deriv*)
Ilicheva, I.A. *et al, Bioorg. Khim.*, 1989, **15**, 800; *Sov. J. Bioorg. Chem. (Engl. Transl.)*, 1989, **15**, 428 (*conformn, anal*)
Horton, D. *et al, Carbohydr. Res.*, 1990, **205**, 71 (*β-pyr deriv, pmr*)

3-Deoxy-3-iodoribose D-1-00065



α-D-Furanose-*form*

$C_5H_9IO_4$ M 260.0

α-D-Furanose-form

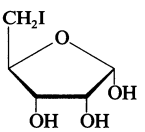
1,2-O-Isopropylidene, 5-methoxycarbonyl: [136317-52-7].
$C_{10}H_{15}IO_6$ M 358.1 Cryst. (hexane). Mp 106-106.5°.

β-L-Pyranose-form

Me glycoside, 2,4-dibenzoyl:
$C_{20}H_{19}IO_6$ M 482.2 Leaflets (EtOH). Mp 143-144°. $[\alpha]_D^{25}$ +55 (c, 1.64 in $CHCl_3$).

Lemieux, R.U. *et al, Can. J. Chem.*, 1969, **47**, 4413 (*β-pyr deriv*)
Japan. Pat., 62 149 697, (1987); *CA*, **108**, 6351k (*deriv*)
Branchaud, B.P. *et al, Organometallics*, 1991, **10**, 3795 (*α-fur deriv*)

5-Deoxy-5-iodoribose D-1-00066



α-D-Furanose-*form*

$C_5H_9IO_4$ M 260.0

α-D-Furanose-form

1,2-O-Isopropylidene: [84258-15-1].
$C_8H_{13}IO_4$ M 300.0 Cryst. (EtOAc/hexane). Mp 84-85°. $[\alpha]_D^{25}$ +20.6 (c, 0.5 in $CHCl_3$).

1,2-O-Isopropylidene, 3-benzyl: [89702-28-3].
$C_{15}H_{19}IO_4$ M 390.2 Oil. $[\alpha]_D^{20}$ +84.9 (c, 4.7 in CH_2Cl_2).

1-(Dihydrogen phosphate): [100752-90-7].
$C_5H_{10}IO_7P$ M 340.0 Syrup.

β-D-Furanose-form

Tri-Ac:
$C_{11}H_{15}IO_7$ M 386.1 Cryst. Mp 86-88°. $[\alpha]_D$ −39 (EtOH).

2,3-Dibenzoyl, 1-Ac: [19945-76-7].
$C_{21}H_{19}IO_7$ M 510.2 Cryst. Mp 112-113°. $[\alpha]_D^{21}$ +20.4 (c, 2.0 in $CHCl_3$).

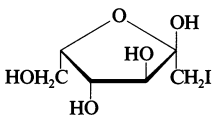
2,3-O-Isopropylidene, 1-Ac: [111570-90-2].
$C_{10}H_{15}IO_5$ M 342.1 Cryst. Mp 38°. $[\alpha]_D^{22}$ −65.8 (c, 0.3 in MeOH).

Me glycoside, 2,3-O-isopropylidene: [38838-06-1].
$C_9H_{15}IO_4$ M 314.1 Syrup. $Bp_{0.1}$ 75-80° (78-79°). $[\alpha]_D^{22}$ −71 (c, 1.0 in $CHCl_3$), $[\alpha]_D^{25}$ −68 ($CHCl_3$).

Me glycoside, 2,3-O-benzylidene: [33208-38-7].
$C_{13}H_{15}IO_4$ M 362.1 Syrup. $[\alpha]_D^{25}$ −42.5 (c, 0.8 in $CHCl_3$).

Pischel, H. *et al, Z. Chem.*, 1968, **8**, 178 (*β-dibenzoyl*)
Prystas, M. *et al, Coll. Czech. Chem. Comm.*, 1971, **36**, 1448 (*β-Me gly*)
Hanessian, S. *et al, Carbohydr. Res.*, 1972, **24**, 45 (*β-Me gly*)
Kiss, J. *et al, Helv. Chim. Acta*, 1982, **65**, 1522 (*α-isopropylidene*)
Ohrui, H. *et al, Agric. Biol. Chem.*, 1987, **51**, 625 (*β-isopropylidene*)
Choi, H.S. *et al, CA*, 1991, **114**, 177971r (*phosphate, synth, metab*)
Furstner, A. *et al, J.O.C.*, 1991, **56**, 2213 (*α-isopropylidene*)

1-Deoxy-1-iodosorbose D-1-00067



$C_6H_{11}IO_5$ M 290.0

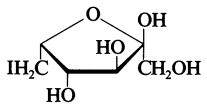
α-L-Furanose-form

2,3-O-Isopropylidene: [38084-09-2].
$C_9H_{15}IO_5$ M 330.1 Cryst. (Et_2O/pentane). Mp 112-113°. $[\alpha]_D^{18}$ −3.1 (c, 1 in $CHCl_3$).

2,3:4,6-Di-O-isopropylidene: [38084-00-3].
$C_{12}H_{19}IO_5$ M 370.1 Cryst. (heptane). Mp 82-83°. $[\alpha]_D^{22}$ −24.5 (c, 1 in $CHCl_3$).

Gardner, T.S. *et al, J.O.C.*, 1947, **12**, 733 (*diisopropylidene*)
James, K. *et al, Aust. J. Chem.*, 1972, **25**, 1967 (α-L-fur derivs, pmr)
Fuerstner, A. *et al, J. Carbohydr. Chem.*, 1990, **9**, 561 (*props, use*)

6-Deoxy-6-iodosorbose D-1-00068



α-L-Furanose-*form*

$C_6H_{11}IO_5$ M 290.0

L-Furanose-form

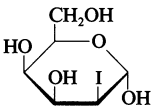
2,3-O-Isopropylidene, 1-tosyl:
$C_{16}H_{21}IO_7S$ M 484.3 Mp 130-140°. $[\alpha]_D$ +25 (EtOH).

α-L-Furanose-form

2,3-O-Isopropylidene, 1-Ac: [58238-55-4].
$C_{11}H_{17}IO_6$ M 372.1 Cryst. (Et_2O/petrol). Mp 106°. $[\alpha]_D^{20}$ +35.8 (c, 1 in $CHCl_3$).

Muller, H. *et al, Helv. Chim. Acta*, 1938, **21**, 263 (*tosyl*)
Heyns, K. *et al, Chem. Ber.*, 1975, **108**, 3619 (*Ac*)

2-Deoxy-2-iodotalose D-1-00069



$C_6H_{11}IO_5$ M 290.0

α-D-Pyranose-form

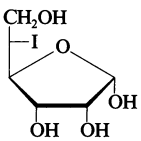
Me glycoside: [53008-83-6].
$C_7H_{13}IO_5$ M 304.0 Syrup.

Me glycoside, tri-Ac: [53008-81-4].
$C_{13}H_{19}IO_8$ M 430.1 Syrup.

Benzyl glycoside, 4,6-O-benzylidene (S-): [75810-26-3].
$C_{20}H_{21}IO_5$ M 468.2 Cryst. (EtOAc/hexane). Mp 138.8°. $[\alpha]_D^{20}$ +110.7 (c, 1 in $CHCl_3$).

Honda, S. *et al, Carbohydr. Res.*, 1974, **34**, 45 (*α-Me gly, pmr*)
Thiem, J. *et al, Chem. Ber.*, 1980, **113**, 3067 (*benzyl gly deriv*)
Korth, H.G. *et al, J.C.S. Perkin 2*, 1986, 1461 (*conformn*)
Chen, S.H. *et al, J.O.C.*, 1991, **56**, 5834 (*α-Me gly tri-Ac, ir, pmr, ms*)

5-Deoxy-5-iodotalose D-1-00070



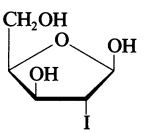
$C_6H_{11}IO_5$ M 290.0

β-L-Furanose-form

1,2-O-Isopropylidene, 3,5-dibenzoyl: [55085-27-3].
$C_{23}H_{23}IO_7$ M 538.3 Cryst. (EtOH). Mp 122-124°. $[\alpha]_D^{20}$ +70 (c, 0.6 in CH_2Cl_2).

Serge, D. *et al, C. R. Hebd. Seances Acad. Sci. Ser. C*, 1974, **279**, 651 (*isopropylidene deriv*)
Serge, D. *et al, Chem. Ber.*, 1979, **77**, 79 (*isopropylidene deriv, pmr*)

2-Deoxy-2-iodoxylose D-1-00071



β-D-Furanose-*form*

$C_5H_9IO_4$ M 260.0

β-D-Furanose-form

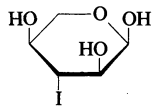
Me glycoside, 3-tosyl, 5-Ac: [26528-13-2].
$C_{15}H_{19}IO_7S$ M 470.2 Cryst. (EtOH). Mp 118-119°. $[\alpha]_D^{25}$ −80.7 (c, 3.4 in $CHCl_3$).

β-L-Pyranose-form

Me glycoside, di-Ac: [131267-51-1].
$C_{10}H_{15}IO_6$ M 358.1 Cryst. (Et_2O/hexane). Mp 110-112°. $[\alpha]_D^{20}$ −49.2 (c, 1.0 in $CHCl_3$).

Lemieux, R.U. *et al, Can. J. Chem.*, 1969, **47**, 4413 (*Me fur deriv*)
Horton, D. *et al, Carbohydr. Res.*, 1990, **205**, 71 (*Me pyr deriv, pmr*)

3-Deoxy-3-iodoxylose D-1-00072



α-L-Pyranose-*form*

$C_5H_9IO_4$ M 260.0

α-L-Pyranose-form

Me glycoside, 4-Ac: [26528-31-4]. $C_8H_{13}IO_5$ M 316.0 Cryst. (EtOH). Mp 125-126°. $[\alpha]_D^{25}$ −109 (c, 2.2 in $CHCl_3$).

Me glycoside, 4-Ac, 2-tosyl: [26532-18-3]. Cryst. (EtOH). Mp 116-117°. $[\alpha]_D^{25}$ −60 (c, 2.5 in $CHCl_3$).

Me glycoside, di-Ac: [26528-32-5]. $C_{10}H_{15}IO_6$ M 358.1 Cryst. Mp 89.5-90.5°.

β-L-Pyranose-form

Me glycoside, 4-Ac: [26528-20-1]. Cryst. (EtOH). Mp 145-145.5°. $[\alpha]_D^{25}$ +10.7 (c, 3.28 in $CHCl_3$).

Me glycoside, 4-Ac, 2-tosyl: [26532-15-0]. Cryst. (EtOH). Mp 131-132.5°. $[\alpha]_D^{25}$ −60 (c, 2.51 in $CHCl_3$).

Me glycoside, di-Ac: [26528-21-2]. Leaflets. Mp 141-141.5°. $[\alpha]_D^{25}$ +39.4 (c, 3.2 in $CHCl_3$).

Me glycoside, 4-benzoyl: [26528-16-5]. $C_{13}H_{15}IO_5$ M 378.1 Needles (EtOH). Mp 158-159°. $[\alpha]_D^{25}$ +113 (c, 1.44 in $CHCl_3$).

Me glycoside, 4-Me: [26528-25-6]. $C_7H_{13}IO_4$ M 288.0 Cryst. (EtOH). Mp 94.5-95.5°.

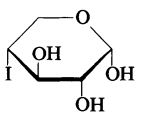
Me glycoside, 4-Me, 2-Ac: [26528-26-7]. $C_9H_{15}IO_5$ M 330.1 Cryst. (EtOH). Mp 125.5-126.5°.

Benzyl glycoside: [128843-81-2]. $C_{12}H_{15}IO_4$ M 350.1 Cryst. (EtOAc/heptane or $CHCl_3$/heptane). Mp 67-70°. $[\alpha]_D^{25}$ −7.6 (c, 1.1 in $CHCl_3$).

Lemieux, R.U. *et al, Can. J. Chem.*, 1969, **47**, 4413 (*Me gly derivs*)

Rehnberg, N. *et al, J.O.C.*, 1990, **55**, 5467 (*benzyl gly*)

4-Deoxy-4-iodoxylose D-1-00073



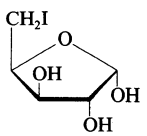
$C_5H_9IO_4$ M 260.0

α-D-Pyranose-form

Benzyl glycoside, 2-benzyl: [50908-55-9]. $C_{19}H_{21}IO_4$ M 440.2 Cryst. Mp 89-91°. $[\alpha]_D$ +130 (c, 1.34 in $CHCl_3$).

Ritchie, R. *et al, Chem. Comm.*, 1973, 686 (*benzyl gly deriv, pmr*)

5-Deoxy-5-iodoxylose D-1-00074



α-D-Furanose-*form*

$C_5H_9IO_4$ M 260.0

α-D-Furanose-form

1,2-O-Isopropylidene: [50600-39-0]. $C_8H_{13}IO_4$ M 300.0 Powder. $[\alpha]_D^{20}$ −38 (c, 1.07 in $CHCl_3$).

1,2-O-Isopropylidene, 3-Ac: [20853-29-6]. $C_{10}H_{15}IO_5$ M 342.1 Syrup.

1,2-O-Isopropylidene, 3-benzoyl: [41164-24-3]. $C_{15}H_{17}IO_5$ M 404.2 Syrup. $[\alpha]_D^{25}$ −50.8 (c, 1.02 in $CHCl_3$).

1,2-O-Isopropylidene, 3-tosyl: [29873-56-1]. $C_{15}H_{19}IO_6S$ M 454.2 Pale yellow syrup. $[\alpha]_D^{23}$ −65.5 (c, 2.0 in $CHCl_3$).

1,2-O-Isopropylidene, 3-benzyl: [29580-99-2]. $C_{15}H_{19}IO_4$ M 390.2 Needles (EtOH). Mp 74-75°. $[\alpha]_D^{23}$ −81.5 (c, 0.68 in $CHCl_3$).

1,2-O-Isopropylidene, 3-trimethylsilyl: [16749-52-3]. $C_{11}H_{21}IO_4Si$ M 372.2 Oil. $Bp_{0.006}$ 72-74°. n_D^{25} 1.4861.

Hedgeley, E.J. *et al, J.C.S.(C)*, 1967, 888 (*trimethylsilyl*)

Ando, H. *et al, Bull. Chem. Soc. Jpn.*, 1970, **43**, 2966 (*tosyl*)

Young, R.C. *et al, Tetrahedron*, 1970, **26**, 3983 (*benzyl*)

Culbertson, T.P., *J.O.C.*, 1973, **38**, 3624 (*benzoyl, pmr*)

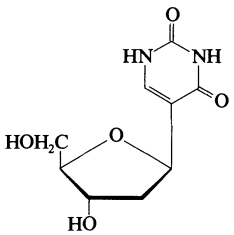
Rahman, A.U. *et al, J. Chem. Soc. Pak.*, 1986, **8**, 397 (*Ac, pmr*)

Achab, S. *et al, J.C.S. Perkin 1*, 1990, 2863 (*isopropylidene, pmr*)

2′-Deoxypseudouridine D-1-00075

*5-(2-Deoxy-β-D-*erythro*-pentofuranosyl)-2,4(1H,3H)-pyrimidinedione, 9CI. 2′-Deoxy-ψ-uridine*

[39967-60-7]



$C_9H_{12}N_2O_5$ M 228.2

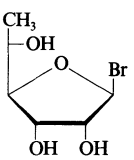
Cryst. (EtOH). Mp 219-221°.

Matsuda, A. *et al, J.O.C.*, 1981, **46**, 3603 (*synth, uv*)

Pankiewicz, K. *et al, J.O.C.*, 1982, **47**, 485 (*synth, pmr*)

Zhang, H.-C. *et al, J.O.C.*, 1992, **57**, 4690 (*synth*)

6-Deoxytalofuranosyl bromide D-1-00076



$C_6H_{11}BrO_4$ M 227.0

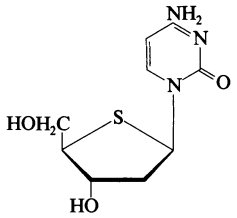
α-L-form

Tris(4-nitrobenzoyl): [80851-32-7]. Yellowish-white cryst. (CH_2Cl_2/hexane). Mp 149° dec.

El Khadem, H.S. *et al, Carbohydr. Res.*, 1981, **98**, 195 (*nitrobenzoyl, ir*)

2′-Deoxy-4′-thiocytidine, 9CI D-1-00077

[134111-30-1]



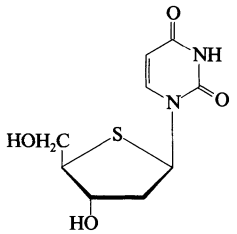
$C_9H_{13}N_3O_3S$ M 243.2

Amorph. powder (EtOH). Mp 129-132°. Hygroscopic.

Secrist, J.A. *et al, J. Med. Chem.*, 1991, **34**, 2361 (*synth, pmr, cmr*)

2′-Deoxy-4′-thiouridine, 9CI D-1-00078

[134111-32-3]



$C_9H_{12}N_2O_4S$ M 244.2

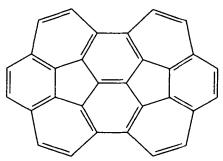
Cryst. (EtOH). Mp 186-188°.

Secrist, J.A. *et al, J. Med. Chem.*, 1991, **34**, 2361 (*synth, uv, pmr, cmr*)

Diacenaphtho[3,2,1,8-*cdefg*:3′,2′,1′,8′-*lmnop*]chrysene D-1-00079

Semibuckminsterfullerene

[158013-82-2]

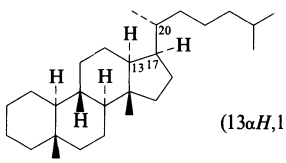


$C_{30}H_{12}$ M 372.4

Bowl-shaped molecule representing half of the skeleton of Fullerene-C_{60}, F-0-01305. Yellow needles. Mp >300° dec.

Rabideau, P.W. *et al, J.A.C.S.*, 1994, **116**, 7891 (*synth, pmr, cmr*)

Diacholestane D-1-00080



(13α*H*,17α*H*,20*R*)-*form*

$C_{27}H_{48}$ M 372.6

(13αH,17αH,20R)-form

Cryst. Mp 85°.

(13αH,17βH,20R)-form

Constit. of petroleum. Oil.

(13αH,17βH,20S)-form

Constit. of petroleum. Oil.

(13βH,17αH,20R)-form
Constit. of petroleum. Oil.

(13βH,17αH,20S)-form
Constit. of petroleum. Cryst. Mp 83.5°.

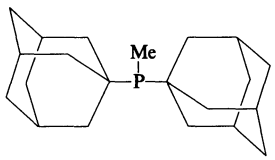
(13βH,17βH,20R)-form
Oil.

Sieskind, O. *et al*, *Tetrahedron*, 1995, **51**, 2009 (*isol, synth, cryst struct, pmr, cmr*)

Di-1-adamantylmethylphosphine D-1-00081

Methyl[bis(tricyclo[3.3.1.1^{3,7}]dec-1-yl)]phosphine

[105944-81-8]



$C_{21}H_{33}P$ M 316.4
Characterised as the oxide.

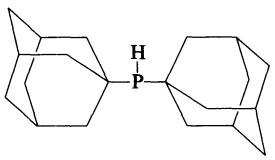
Oxide: [154147-28-1].
$C_{21}H_{33}OP$ M 332.4 Solid. Mp 155° dec.

Goerlich, J.R. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1993, **81**, 141 (*synth, deriv, ms, pmr, P-31 nmr*)

Di-1-adamantylphosphine D-1-00082

Bis(bicyclo[3.3.1.1^{3,7}]dec-1-yl)phosphine

[131211-27-3]



$C_{20}H_{31}P$ M 302.4
Ligand for Ni, Fe, Cr, Mo and W. Cryst. (MeCN/Et_2O). Mp 134-137°, Mp 174-176°.

Methiodide: Di-1-adamantyl(methyl)phosphonium iodide
$C_{21}H_{34}IP$ M 444.3 Solid. Mp >240°.

Oxide: [131266-79-0].
$C_{20}H_{31}OP$ M 318.4 Cryst. (Et_2O). Mp 255-258° (251°).

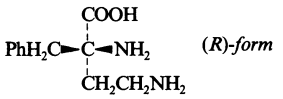
Sulfide: [154147-23-6].
$C_{20}H_{31}PS$ M 334.5 Golden brown cryst. Mp 142°.

Selenide: [154147-25-8].
$C_{20}H_{31}PSe$ M 381.3 Solid. Mp 241°.

No, B.I. *et al*, *Zh. Obshch. Khim.*, 1990, **60**, 1795; *J. Gen. Chem. USSR (Engl. Transl.)*, 1990, **60**, 1603 (*synth, oxide*)
Goerlich, J.R. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1993, **81**, 141 (*synth, derivs, ms, pmr, P-31 nmr*)
Goerlich, J.R. *et al*, *Polyhedron*, 1993, **12**, 2279 (*complexes*)
Goerlich, J.R. *et al*, *Z. Naturforsch., B*, 1994, **49**, 801 (*oxide*)
Lavrova, E.A. *et al*, *Zh. Obshch. Khim.*, 1994, **64**, 1556; *J. Gen. Chem. USSR (Engl. Transl.)*, 1994, **64**, 1393 (*synth, P-31 nmr*)

2,4-Diamino-2-benzylbutanoic acid D-1-00083

α-(2-Aminoethyl)phenylalanine, 9CI



(*R*)-*form*

$C_{11}H_{16}N_2O_2$ M 208.2
(*R*)-*form* [159801-69-1]
D-*form*

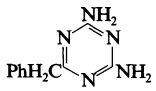
Dihydrochloride: Cryst. (EtOH/dioxan). Mp 154° dec.

Cheng, H. *et al*, *J.O.C.*, 1994, **59**, 7671 (*synth, ir, pmr*)

2,4-Diamino-6-benzyl-1,3,5-triazine D-1-00084

6-(Phenylmethyl)-1,3,5-triazine-2,4-diamine, 9CI. 6-Benzylguanamine. Phenylacetoguanamine

[1853-88-9]



$C_{10}H_{11}N_5$ M 201.2
Flame retardant, stabiliser of aq. formaldehyde solns. and urethane polymer coatings. Cryst. (EtOH). Mp 245° (238-299°).

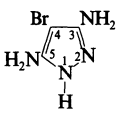
Hydrochloride: Cryst. (EtOH/Et_2O). Mp 215°.
Sulfate (1:1): Cryst. Mp 193-203°.
Sulfate (2:1): Cryst. + $2H_2O$. Mp 254° (178-183°).
Picrate: Yellow cryst. Mp 267-268° (235° dec.).
N-*Ac:*
$C_{12}H_{13}N_5O$ M 243.2 Cryst. (EtOH). Mp 248° (239-240°).
2N,4N-*Di-Ac:*
$C_{14}H_{15}N_5O_2$ M 285.3 Yellow cryst. (EtOAc). Mp 145°.

Ostrogovich, A.E. *et al*, *Gazz. Chim. Ital.*, 1930, **60**, 648 (*synth*)
Ger. Pat., 965 489, (1957); *CA*, **53**, 14010b (*synth, deriv*)
U.S. Pat., 2 792 395, (1957); *CA*, **51**, 14837h (*synth, deriv*)
Italian Pat., 805 928, (1968); *CA*, **71**, 38350t (*use*)
Japan. Pat., 6 909 828, (1969); *CA*, **71**, 114302w (*use*)
Eur. Pat., 14 463, (1980); *CA*, **93**, 221539e (*use*)

3,5-Diamino-4-bromo-1*H*-pyrazole D-1-00085

4-Bromo-1H-pyrazole-3,5-diamine

[16675-36-8]



$C_3H_5BrN_4$ M 177.0
Cryst. (EtOH/Et_2O). Mp 135-136° dec.

Settepani, J.A. *et al*, *J.O.C.*, 1968, **33**, 2606 (*synth, ir, uv*)

1,4-Diamino-2-butanone, 9CI, 8CI D-1-00086

$H_2NCH_2CH_2COCH_2NH_2$

$C_4H_{10}N_2O$ M 102.1
Inhibitor of pea diamine oxidase.

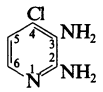
Hydrochloride (1:2): [3660-09-1]. Cryst. (EtOH). Mp 220-221° (215-216°) dec.
Hydrobromide (1:2): Cryst. Mp 230-231° dec.
Picrate: Yellow cryst. Mp 212° dec.
N,N′-*Diphthalimido:*
$C_{20}H_{14}N_2O_5$ M 362.3 Plates (AcOH). Mp 248-249°.

Aldrich Library of FT-IR Spectra, 1st edn., **1**, 460B.
Aldrich Library of NMR Spectra, 2nd edn., **1**, 384D.
Pyman, L., *J.O.C.*, 1930, 99 (*synth*)
Fraser, M.R. *et al*, *J.C.S.*, 1952, 226 (*synth*)
Korobitsyana, I.K. *et al*, *Zh. Obshch. Khim.*, 1956, **26**, 1660; *J. Gen. Chem. USSR (Engl. Transl.)*, 1956, **26**, 1861 (*deriv*)
Vitali, T. *et al*, *CA*, 1984, **100**, 97196n (*synth*)
Macholan, L. *et al*, *Coll. Czech. Chem. Comm.*, 1991, **56**, 1545 (*biochem*)

2,3-Diamino-4-chloropyridine D-1-00087

4-Chloro-2,3-pyridinediamine

[24484-98-8]



$C_5H_6ClN_3$ M 143.5
Needles (H_2O). Mp 158-159°.

De Roos, K.B. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1969, **88**, 1263 (*synth, ir, uv*)

2,3-Diamino-5-chloropyridine D-1-00088

5-Chloro-2,3-pyridinediamine, 9CI

[25710-20-7]

$C_5H_6ClN_3$ M 143.5
Needles (H_2O). Mp 174-176°.

Vaughan, J.R. *et al*, *J.A.C.S.*, 1949, **71**, 1885 (*synth*)
Ziegler, J.B., *J.A.C.S.*, 1949, **71**, 1891 (*synth*)
Takahashi, T. *et al*, *Chem. Pharm. Bull.*, 1958, **6**, 443 (*synth*)

2,3-Diamino-6-chloropyridine D-1-00089

6-Chloro-2,3-pyridinediamine, 9CI

[40851-95-4]

$C_5H_6ClN_3$ M 143.5
Needles (H_2O or C_6H_6). Mp 132-133°.

[40851-88-5]

Tschitschibabin, A.E. *et al*, *Ber.*, 1927, **60**, 766 (*synth*)

2,6-Diamino-4-chloropyridine D-1-00090

4-Chloro-2,6-pyridinediamine, 9CI

[6309-00-8]

$C_5H_6ClN_3$ M 143.5
Cryst. (C_6H_6). Mp 102.5°.

Markees, D.G. *et al*, *J.A.C.S.*, 1956, **78**, 4130 (*synth*)

3,4-Diamino-2-chloropyridine D-1-00091

2-Chloro-3,4-pyridinediamine, 9CI

[39217-08-8]

$C_5H_6ClN_3$ M 143.5
Cryst. (EtOH). Mp 155°.

Dihydrochloride: Cryst. Mp 175-177°.

Talik, Z. *et al, Rocz. Chem.*, 1956, **30**, 1139 (*synth*)
Rousseau, R.J. *et al, J. Het. Chem.*, 1965, **2**, 196 (*synth*)
Dvorakova, H. *et al, Coll. Czech. Chem. Comm.*, 1993, **58**, 629 (*synth*)

3,5-Diamino-2-chloropyridine D-1-00092

2-Chloro-3,5-pyridinediamine

$C_5H_6ClN_3$ M 143.5
Cryst. Mp 101-103°.

Tomasik, P. *et al, Rocz. Chem.*, 1965, **39**, 1671 (*synth*)

4,5-Diamino-2-chloropyridine D-1-00093

6-Chloro-3,4-pyridinediamine

$C_5H_6ClN_3$ M 143.5
Cryst. (C_6H_6). Mp 146°.

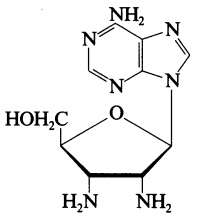
Hydrochloride: Cryst. (EtOH/Et_2O). Mp 238-239°.

Talik, Z. *et al, Rocz. Chem.*, 1956, **30**, 1139 (*synth*)
Albert, A. *et al, J.C.S.*, 1963, 5156 (*synth*)
Rousseau, R.J. *et al, J. Het. Chem.*, 1965, **2**, 196 (*synth*)

2′,3′-Diamino-2′,3′-dideoxyadenosine, 9CI D-1-00094

9-(2,3-Diamino-2,3-dideoxy-β-D-ribofuranosyl) adenine

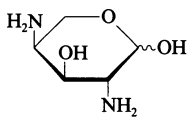
[90362-10-0]



$C_{10}H_{15}N_7O_2$ M 265.2
Needles (MeOH/Et_2O). Mp *ca.* 175° (softens at *ca.* 155°).

Chen, Y.-C.J. *et al, J.O.C.*, 1991, **56**, 3410 (*synth, pmr, ms*)

2,4-Diamino-2,4-dideoxyarabinose D-1-00095



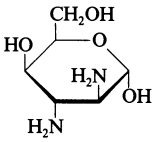
L-Pyranose-*form*

$C_5H_{12}N_2O_3$ M 148.1

L-form [135221-06-6]
Pt complexes used as antitumour agents. Inhibits mice leukaemia (L-1210). Syrup.

Japan. Pat., 90 223 591, (1990); *CA*, **115**, 84232f (*activity*)

2,3-Diamino-2,3-dideoxyidose D-1-00096



$C_6H_{14}N_2O_4$ M 178.1

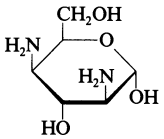
α-D-Pyranose-form

Me glycoside, 2N,3N-di-Ac: [88261-56-7].
$C_{11}H_{20}N_2O_6$ M 276.2 Cryst. (EtOH). Mp 220-221°. $[\alpha]_D^{20}$ +74 (c, 1 in H_2O).

Me glycoside, 4,6-O-benzylidene, 2N,3N-di-Ac: [52885-53-7].
$C_{18}H_{24}N_2O_6$ M 364.3 Cryst. Mp 304-305°. $[\alpha]_D$ +39 (c, 0.7 in $CHCl_3$).

Guthrie, R.D. *et al, J.C.S. Perkin 1*, 1974, 650 (*α-Me pyr benzylidene*)
Knivel, Y.A. *et al, Carbohydr. Res.*, 1983, **122**, 181 (*α-Me pyr, di-Ac, cmr*)

2,4-Diamino-2,4-dideoxyidose D-1-00097



$C_6H_{14}N_2O_4$ M 178.1

α-D-Pyranose-form

Me glycoside: [58645-30-0].
$C_7H_{16}N_2O_4$ M 192.2 Syrup. $[\alpha]_D^{20}$ +74 (c, 5.4 in H_2O).

Me glycoside, 2N,4N-di-Ac: [29788-86-1].
$C_{11}H_{20}N_2O_6$ M 276.2 Cryst. (EtOH). Mp 242-244°. $[\alpha]_D^{22}$ +61 (c, 0.2 in H_2O).

Me glycoside, 2N,3,4N,6-tetra-Ac: [29788-85-0].
$C_{15}H_{24}N_2O_8$ M 360.3 Cryst. (EtOH). Mp 245-247°. $[\alpha]_D^{22}$ +80 (c, 1 in H_2O).

Me glycoside, 2N,3,4N,4N,6-penta-Ac: [58645-26-4].
$C_{17}H_{26}N_2O_9$ M 402.4 Syrup. $[\alpha]_D^{20}$ +24 (c, 2 in MeOH).

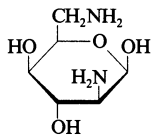
Me glycoside, 3,6-dibenzoyl, 2N,4N-di-Ac: [58645-24-2].
$C_{25}H_{28}N_2O_8$ M 484.5 Cryst. (EtOH). Mp 263-265°. $[\alpha]_D^{20}$ +52 (c, 2 in $CHCl_3$).

Me glycoside, 2N,3,4N,6-tetrabenzoyl, 2N,4N-di-Ac:
$C_{39}H_{36}N_2O_{10}$ M 692.7 Cryst.

Me glycoside, 3,6-di-Me, 2N,4N-di-Ac: [58645-32-2].
$C_{13}H_{24}N_2O_6$ M 304.3 Cryst. (EtOH). Mp 248-250°. $[\alpha]_D^{20}$ +91 (c, 4 in MeOH).

Suami, T. *et al, Bull. Chem. Soc. Jpn.*, 1970, **43**, 2948 (*Me gly derivs*)
Paulsen, H. *et al, Carbohydr. Res.*, 1975, **45**, 205 (*Me gly derivs, pmr, conformn*)
Luger, P. *et al, Acta Cryst. B*, 1978, **34**, 1254 (*tetrabenzoyl, cryst struct*)

2,6-Diamino-2,6-dideoxyidose D-1-00098



β-D-Pyranose-*form*

$C_6H_{14}N_2O_4$ M 178.1

D-form

Hydrochloride: [51250-07-8].
Syrup.

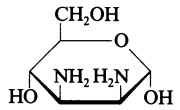
β-D-Pyranose-form

Me glycoside, 2N-Ac: [59150-47-9].
$C_9H_{17}N_2O_5$ M 233.2 Cryst. (EtOAc/petrol). Mp 149-153°. $[\alpha]_D^{20}$ −108 (c, 1.0 in H_2O).

Me glycoside, 2N,3,4-tri-Ac: [59150-46-8].
$C_{13}H_{21}N_2O_7$ M 317.3 Cryst. (EtOAc/petrol). Mp 140-144°. $[\alpha]_D^{20}$ −37 (c, 1.0 in $CHCl_3$).

Perry, M.B. *et al, Can. J. Biochem.*, 1973, **51**, 1335 (D-form, chromatogr)
Jaroslavi, S. *et al, Coll. Czech. Chem. Comm.*, 1975, **40**, 3698 (*β-Me pyr deriv, pmr*)

2,3-Diamino-2,3-dideoxymannose D-1-00099



α-D-Pyranose-*form*

$C_6H_{14}N_2O_4$ M 178.1
Pt complexes exhibit antitumour activity.

D-Pyranose-form

Hydrochloride: [21871-07-8].
Cryst. (EtOH/EtOAc). $[\alpha]_D$ +1 (2 min.) → −3 (1h) (c, 0.6 in H_2O).

α-D-Pyranose-form

Me glycoside, 2N,3N-di-Ac: [53840-71-4].
$C_{11}H_{20}N_2O_6$ M 276.2 Cryst. Mp 248-250°. $[\alpha]_D$ +4.8 (c, 0.4 in H_2O).

Me glycoside, 2N,3N,4,6-tetra-Ac: [6386-22-7].
$C_{15}H_{24}N_2O_8$ M 360.3 Cryst. (C_6H_6/petrol). Mp 200-202°. $[\alpha]_D$ +89.2 ($CHCl_3$).

Me glycoside, 4,6-O-benzylidene, 2N,3N-di-Ac: [3150-18-3].
$C_{18}H_{24}N_2O_6$ M 364.3 Cryst. Mp 310-311°. $[\alpha]_D$ −36.2 (DMF).

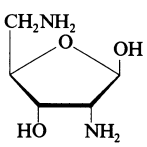
β-D-Pyranose-form

Me glycoside: [21871-05-6].
$C_7H_{16}N_2O_4$ M 192.2 Cryst. + 0.66 2-propanol (MeOH/2-propanol) (as dihydrochloride). Mp 180° dec. (browns) (dihydrochloride). $[\alpha]_D$ −46.7 (c, 1 in H_2O). CAS no. refers to dihydrochloride.

Me glycoside, 2N,3N-di-Ac: [21871-06-7].
Cryst. Mp 116-135°. $[\alpha]_D$ −108 (c, 0.6 in H_2O).

Guthrie, R.D. *et al, Chem. Ind. (London)*, 1962, 1473 (*α-Me pyr benzylidene di-Ac*)
Baer, H.H. *et al, J.O.C.*, 1969, **34**, 3848 (*synth, β-Me pyr derivs, ir*)
Baer, H.H. *et al, Can. J. Chem.*, 1974, **52**, 2257 (*α-Me pyr acetates, ir*)
Tsubomura, T. *et al, Chem. Comm.*, 1986, 459 (*Pt complexes, pharmacol*)

2,5-Diamino-2,5-dideoxyribose D-1-00100



β-D-Furanose-*form*

$C_5H_{12}N_2O_3$ M 148.1

D-Furanose-form

2N,5N-Di-Ac: [86258-84-6].
$C_9H_{16}N_2O_5$ M 232.2 Needles. Mp 151-153°. $[\alpha]_D^{20}$ −16 (c, 0.5 in MeOH).

β-D-Furanose-form

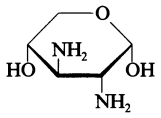
Benzyl glycoside, 2N,5N-di-Ac: [74593-06-9].
$C_{16}H_{22}N_2O_5$ M 322.3 Cryst. Mp 135°. $[\alpha]_D^{20}$ −52 (c, 0.5 in MeOH).

Benzyl glycoside, 2N,3,5N-tri-Ac: [74593-07-0].
$C_{18}H_{24}N_2O_6$ M 364.3 Needles. Mp 160°. $[\alpha]_D^{20}$ −48 (c, 0.2 in MeOH).

[86258-85-7]

Hasegawa, A. *et al, Carbohydr. Res.*, 1980, **81**, 23 (D-fur deriv, β-D-fur deriv, ir, pmr)

2,3-Diamino-2,3-dideoxyxylose D-1-00101



α-D-Pyranose-*form*

$C_5H_{12}N_2O_3$ M 148.1

D-Pyranose-form

2N,3N-Di-Ac: [79974-86-0].
$C_9H_{16}N_2O_5$ M 232.2 Syrup. $[\alpha]_D^{20}$ −81.22 (c, 0.25 in H_2O).

1,2N,3N,4-Tetra-Ac: [79974-87-1].
$C_{13}H_{20}N_2O_7$ M 316.3 Syrup. $[\alpha]_D^{20}$ +20 (c, 0.1 in $CHCl_3$).

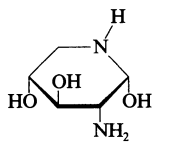
α-D-Pyranose-form

Benzyl pyranoside, 4-benzyl, 2N,3N-di-Ac: [79974-85-9].
$C_{23}H_{28}N_2O_5$ M 412.4 Cryst. ($CHCl_3$/petrol). Mp 256.5°. $[\alpha]_D^{20}$ +62.5 (c, 0.5 in $CHCl_3$).

[79974-96-2, 79974-97-3]

Paulsen, H. *et al, Annalen*, 1981, 1633 (D-pyr deriv, α-D-pyr deriv, pmr)

2,5-Diamino-2,5-dideoxyxylose D-1-00102



α-D-Pyranose-*form*

$C_5H_{12}N_2O_3$ M 148.1

α-D-Pyranose-form

2N,5N-Di-Ac: [86204-37-7].
$C_9H_{16}N_2O_5$ M 232.2 Needles (MeOH). Mp 190-192° dec. $[\alpha]_D^{20}$ +17 (c, 0.38 in MeOH).

1,2N,3,4,5N-Penta-Ac: [86204-38-8].
$C_{15}H_{22}N_2O_8$ M 358.3 Prisms. Mp 178-179°. $[\alpha]_D^{20}$ +30 (c, 0.25 in $CHCl_3$).

D-Furanose-form

2N,5N-Di-Ac: [86258-82-4].
Needles (EtOH/Et_2O). Mp 171°. $[\alpha]_D^{26}$ +64 (c, 0.5 in MeOH).

α-D-Furanose-form

1,2N,3,5N-Tetra-Ac:
$C_{13}H_{20}N_2O_7$ M 316.3 Needles. Mp 198-200° dec. $[\alpha]_D^{20}$ +108 (c, 0.3 in MeOH).

β-D-Furanose-form

Benzyl glycoside, 2N,5N-di-Ac: [74593-38-7].
$C_{16}H_{22}N_2O_5$ M 322.3 Needles (EtOH). Mp 249° dec. $[\alpha]_D^{20}$ −62 (c, 0.3 in MeOH).

Benzyl glycoside, 2N,3,5N-tri-Ac:
$C_{18}H_{24}N_2O_6$ M 364.3 Cryst. (Et_2O). Mp 182-183°. $[\alpha]_D^{20}$ −43 (c, 0.3 in MeOH).

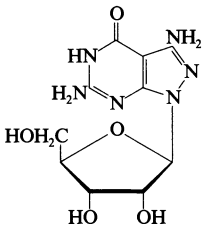
[86286-44-4]

Hasegawa, A. *et al, Carbohydr. Res.*, 1980, **81**, 23 (α-D-fur deriv, benzyl β-D-fur deriv, ir, pmr)

Okumura, H. *et al, Agric. Biol. Chem.*, 1983, **47**, 839 (D-fur deriv, α-D-pyr deriv, ir, pmr)

3,6-Diamino-1,5-dihydro-1-β-D-ribofuranosyl-4*H*-pyrazolo[3,4-*d*]pyrimidin-4-one, 9CI D-1-00103

[127820-69-3]

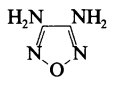


$C_{10}H_{14}N_6O_5$ M 298.2
Solid. Mp 180° dec.

Bontems, R.J. *et al, J. Med. Chem.*, 1990, **33**, 2174 (*synth, uv, pmr*)

Diaminofurazan D-1-00104

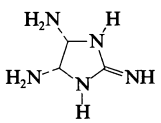
Furazandiamine



$C_2H_4N_4O$ M 100.0
Needles. Mp 180°.

Gunasekaran, A. *et al, J. Het. Chem.*, 1995, **32**, 1405 (***synth***, *pmr, cmr*)

4,5-Diamino-2-iminoimidazoline D-1-00105



$C_3H_9N_5$ M 115.1

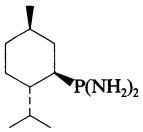
(4RS,5SR)-form

cis-*form*
Cryst. (as trihydrochloride). Mp 215° dec. (trihydrochloride). Discolours above 195° (trihydrochloride).

Dagley, I.J. *et al, Aust. J. Chem.*, 1994, **47**, 2033 (*synth, ir, pmr, cmr, cryst struct*)

3-(Diaminophosphinoyl)-*p*-menthane D-1-00106

P-[*5-Methyl-2-(1-methylethyl)cyclohexyl*] *phosphonous diamide, 9CI.* P-(*2-Isopropyl-5-methylcyclohexyl*)*phosphonous diamide*



$C_{10}H_{23}N_2P$ M 202.2

(1R,2S,5R)-form

P-*Menthylphosphonous diamide*

N,N,N′,N′-*Tetra-Me:* [83021-28-7]. P-(*2-Isopropyl-5-methylcyclohexyl*)-N,N,N′,N′-*tetramethylphosphonous diamide.* P-(*L-Menthyl*)-N,N,N′,N′-*tetramethylphosphonous diamide*
$C_{14}H_{31}N_2P$ M 258.3 Liq. $Bp_{0.01}$ 81°. $[\alpha]_D$ −96.6 (c, 15.23 in C_6H_6).

N,N,N′,N′-*Tetra-Et:* [123973-39-7].
$C_{18}H_{39}N_2P$ M 314.4 Ligand for Cr, Mo, W. Liq. $Bp_{0.005}$ 105-108°.

N,N,N′,N′-*Tetrabutyl:* [131369-80-7].
N,N,N′,N′-*Tetrabutyl*-P-(*2-isopropyl-5-methylcyclohexyl*)*phosphonous diamide.* N,N,N′,N′-*Tetrabutyl*-P-(*L-menthyl*) *phosphonous diamide*
$C_{26}H_{55}N_2P$ M 426.7 Liq. $Bp_{0.005}$ 160°. $[\alpha]$ −33.03 (c, 30 in C_6H_6).

Hidai, M. *et al, J. Organomet. Chem.*, 1982, **232**, 89 (*tetra-Me, synth, pmr*)

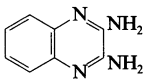
Diemert, K. *et al, J. Organomet. Chem.*, 1989, **378**, 17 (*synth, ms, P-31 nmr, complexes*)

Diemert, K., *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1990, **53**, 339 (*synth, ms, P-31 nmr*)

2,3-Diaminoquinoxaline D-1-00107

2,3-Quinoxalinediamine

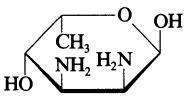
[6640-47-7]



$C_8H_8N_4$ M 160.1
Fine cryst. Mp 331°, Mp >340°.

Obafemi, C.A. *et al, Helv. Chim. Acta*, 1994, **77**, 1549 (*synth, uv, pmr*)

2,3-Diamino-2,3,6-trideoxygulose D-1-00108



$C_6H_{14}N_2O_3$ M 162.1

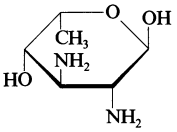
α-L-Pyranose-form

Me glycoside: [81905-75-1].
$C_7H_{16}N_2O_3$ M 176.2 Cryst. Mp 221-222°. $[\alpha]_D$ −97 (c, 1.2 in MeOH).

Me glycoside, 3N-benzyl: [81905-73-9].
$C_{14}H_{22}N_2O_3$ M 266.3 Needles (EtOAc/petrol). Mp 130-131°. $[\alpha]_D$ −93 (c, 1.75 in $CHCl_3$).

Hajivarnava, G.S. *et al, J.C.S. Perkin 1*, 1982, 205 (*α-Me pyr deriv, ir, pmr*)

2,3-Diamino-2,3,6-trideoxyidose D-1-00109



$C_6H_{14}N_2O_3$ M 162.1

α-L-Pyranose-form

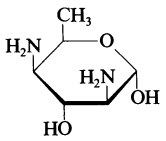
Me glycoside: [81905-74-0].
$C_7H_{16}N_2O_3$ M 176.2 Needles. Mp 199-200°. $[\alpha]_D$ −96 (c, 0.9 in MeOH).

Me glycoside, 3N-benzyl: [81905-72-8].
$C_{14}H_{22}N_2O_3$ M 266.3 Syrup. $[\alpha]_D$ −87 (c, 1.15 in $CHCl_3$).

Me glycoside, 3N-Me: [81905-77-3].
$C_8H_{18}N_2O_3$ M 190.2 Syrup. $[\alpha]_D$ −100 (c, 1.5 in $CHCl_3$).

Hajivarnava, G.S. *et al, J.C.S. Perkin 1*, 1982, 205 (*α-Me pyr deriv, ir, pmr*)

2,4-Diamino-2,4,6-trideoxyidose D-1-00110



α-D-Pyranose-*form*

$C_6H_{14}N_2O_3$ M 162.1

α-D-Pyranose-form

Me glycoside: [58394-13-1].
$C_7H_{16}N_2O_3$ M 176.2 Syrup. $[\alpha]_D^{20}$ +91 (c, 2.4 in MeOH).

Me glycoside, hydrochloride (1:2): [58394-17-5].
Amorph. solid. $[\alpha]_D^{20}$ +65 (c, 2 in H_2O).

Me glycoside, 3-Ac: [58394-19-7].
$C_9H_{18}N_2O_4$ M 218.2 Syrup (as dihydrochloride). $[\alpha]_D^{20}$ +49 (c, 2 in H_2O). CAS no. refers to dihydrochloride.

Me glycoside, 2N,4N-di-Ac: [58394-14-2].
$C_{11}H_{20}N_2O_5$ M 260.2 Cryst. (EtOH). Mp 251°. $[\alpha]_D^{20}$ +65 (c, 2 in MeOH).

Me glycoside, 2N,3,4N-tri-Ac: [58394-10-8].
$C_{13}H_{22}N_2O_6$ M 302.3 Cryst. (EtOH). Mp 246-248°. $[\alpha]_D^{20}$ +38 (c, 2 in MeOH).

L-Pyranose-form

2N,4N-Di-Ac: [50611-21-7].
$C_{10}H_{18}N_2O_5$ M 246.2 Cryst. (EtOH/petrol). Mp 172-174°. $[\alpha]_D^{25}$ −45 (c, 0.87 in H_2O).

α-L-Pyranose-form

Me glycoside, 2N,3,4N-tri-Ac: [34388-74-4]. Needles (EtOAc). Mp 261° dec. $[\alpha]_D^{22}$ −60 (c, 0.38 in $CHCl_3$).

β-L-Pyranose-form

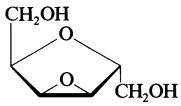
Benzyl glycoside, 2N,4N-di-Ac: [50611-17-1].
$C_{17}H_{24}N_2O_5$ M 336.3 Cryst. (Me_2CO/petrol). Mp 232-233°. $[\alpha]_D^{25}$ +105 (c, 1.1 in MeOH).

Benzyl glycoside, 2N,3,4N-tri-Ac: [50611-15-9].
$C_{19}H_{26}N_2O_6$ M 378.4 Cryst. (Me_2CO/petrol). Mp 193-194°. $[\alpha]_D^{25}$ +70 (c, 1.1 in $CHCl_3$).

Benzyl glycoside, 3-mesyl, 2N,4N-di-Ac: [50611-18-2].
$C_{18}H_{26}N_2O_7S$ M 414.4 Cryst. (EtOH/petrol). Mp 248°. $[\alpha]_D^{25}$ +28 (c, 0.7 in $CHCl_3$).

Zehavi, U. *et al, J.O.C.*, 1972, **37**, 2145 (α-L-pyr deriv)
Liav, A. *et al, Carbohydr. Res.*, 1973, **30**, 109 (L-pyr deriv, β-L-pyr deriv, pmr)
Paulsen, H. *et al, Chem. Ber.*, 1976, **109**, 90 (α-D-pyr deriv)
Capek, K. *et al, Coll. Czech. Chem. Comm.*, 1987, **52**, 2248 (α-D-Me pyr di-Ac, pmr)

2,5:3,4-Dianhydroaltritol D-1-00111



D-*form*

$C_6H_{10}O_4$ M 146.1

D-form [84518-62-7]
Cryst. (EtOH/Et_2O). Mp 91.5-93°. $[\alpha]_D^{24}$ −76.3 (c, 2.73 in MeOH).

1,6-Di-Ac: [84447-11-0].
$C_{10}H_{14}O_6$ M 230.2 Oil. $[\alpha]_D^{25}$ −53.5 (in $CHCl_3$). Incorrectly named as a D-allitol deriv. in the lit.

1,6-Dibenzoyl: [91318-12-6].
$C_{20}H_{18}O_6$ M 354.3 Cryst. (pentane). Mp 73-74°. $[\alpha]_D^{24}$ −70.9 (c, 1.92 in $CHCl_3$).

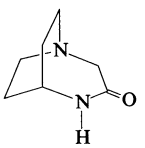
L-form
Syrup. $[\alpha]_D^{20}$ +85.6 (c, 0.9 in EtOH).

DL-form [128899-69-4]
Syrup.

Guthrie, R.D. *et al, Aust. J. Chem.*, 1982, **35**, 2169 (*di-Ac, cmr*)
Otero, D.A. *et al, Carbohydr. Res.*, 1984, **128**, 79 (*synth*, D-form, dibenzyl)
Bock, K. *et al, Acta Chem. Scand.*, 1989, **43**, 264 (*synth*, L-form, pmr)
Kammerer, J. *et al, Angew. Chem., Int. Ed.*, 1990, **29**, 1038 (DL-form)
Gabriel Garcia, J. *et al, Acta Cryst. C*, 1992, **48**, 1692 (*cryst struct*)

1,4-Diazabicyclo[3.2.2]nonan-3-one, 9CI D-1-00112

[53619-11-7]

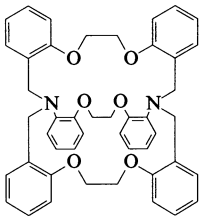


$C_7H_{12}N_2O$ M 140.1

(±)-form
Cryst. (2-propanol). Mp 218-219° (209-211°).

Rubstov, M.V. *et al, Zh. Obshch. Khim.*, 1964, **34**, 2222; *J. Gen. Chem. USSR (Engl. Transl.)*, 1964, **34**, 2232 (*synth*)
Mikhlina, E.E. *et al, Zh. Org. Khim.*, 1965, **1**, 1336; *J. Org. Chem. USSR (Engl. Transl.)*, 1965, **1**, 1352.
de Costa, B.R. *et al, J. Med. Chem.*, 1993, **36**, 2311 (*synth, pmr*)

1,20-Diaza-9,17,28,31,45,48-hexaoxanonacyclo [18.18.18.0^{3,8}.0^{13,18}.0^{22,27}.0^{32,37}.0^{39,44}.0^{49,54}] hexatetraconta-3,5,7,13,15,17,22,24,26,32,34,36,39,41,43,49,51,53-octadecaene D-1-00113

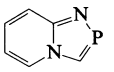


$C_{46}H_{44}N_2O_6$ M 720.8
Microcryst. solid.

Atkinson, I.M. *et al, Aust. J. Chem.*, 1994, **47**, 1155 (*synth, pmr, cmr, cryst struct*)

1,4,2-Diazaphospholo[4,5-*a*] pyridine D-1-00114

[107700-34-5]



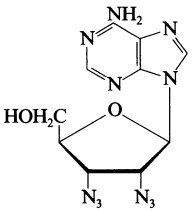
$C_6H_5N_2P$ M 136.0
Pale yellow microcryst. powder with naphthalene-like odour. Mp 44-46°. Reactive to protic nucleophiles.

Karaghiosoff, K. *et al, Phosphorus Sulfur Relat. Elem.*, 1986, **28**, 289 (*synth, P-31 nmr, reaction*)
Litvinov, A. *et al, Heteroat. Chem.*, 1991, **2**, 369 (*synth, pmr, cmr, P-31 nmr, props*)
Wrackmeyer, B. *et al, Magn. Reson. Chem.*, 1991, **29**, 1045 (*cmr, N-15 nmr, P-31 nmr*)

2′,3′-Diazido-2′,3′-dideoxyadenosine, 9CI D-1-00115

9-(2,3-Diazido-2,3-dideoxy-β-D-ribofuranosyl) adenine

[119644-21-2]



$C_{10}H_{11}N_{11}O_2$ M 317.2
Granular solid. Mp 171-172° dec.

Chen, Y.-C.J. *et al, J.O.C.*, 1991, **56**, 3410 (*synth, uv, pmr, ms*)

3-Diazo-2-butanone, 9CI D-1-00116

Azibutanone

[14088-58-5]

$N_2{=}C(CH_3)COCH_3$

$C_4H_6N_2O$ M 98.1
Yellow oil. Bp_{90} 87-89°.

Diels, O. *et al*, *Ber.*, 1915, **58**, 223 (*synth*)
Taber, D.F. *et al*, *J.O.C.*, 1995, **60**, 2283 (*synth, pmr, cmr, ir*)

Diazo(diethoxyphosphinyl) acetic acid D-1-00117

[108764-27-8]

$(EtO)_2P(O)C(N_2)COOH$

$C_6H_{11}N_2O_5P$ M 222.1

Me ester: [96854-79-4]. *Methyl diazo(diethoxyphosphinyl)acetate*
$C_7H_{13}N_2O_5P$ M 236.1 Yellowish oil. d_4^{20} 1.20. Bp_1 98-99°. n_D^{20} 1.4477.

Et ester: [17507-56-1]. *Triethyl diazophosphonoacetate*
$C_8H_{15}N_2O_5P$ M 250.1 Yellow oil. d_4^{20} 1.18. Bp_1 104-106°, $Bp_{0.05}$ 76-80°. n_D^{20} 1.4584.

Amide: Diazo(diethoxyphosphinyl)acetamide
$C_6H_{12}N_3O_4P$ M 221.1 Stable, yellow liq. d_4^{20} 1.24. n_D^{20} 1.4748.

Nitrile: Diazo(diethoxyphosphinyl)acetonitrile
$C_6H_{10}N_3O_3P$ M 203.1 Yellow oil. d_4^{20} 1.21. n_D^{20} 1.4680.

tert-*Butyl ester:* [86394-47-0]. tert-*Butyl diazo(diethoxyphosphinyl)acetate*
$C_{10}H_{19}N_2O_5P$ M 278.2 Red-brown oil.

Petzold, G. *et al*, *Naturwissenschaften*, 1967, **54**, 469 (*synth*)
Khokhlov, P.S. *et al*, *Zh. Obshch. Khim.*, 1984, **54**, 2641, 2785; 1985, **55**, 2254; *J. Gen. Chem. USSR (Engl. Transl.)*, 1984, **54**, 2359, 2495; 1985, **55**, 2002 (*synth, ir, uv, pmr*)
Shiraki, C. *et al*, *Synthesis*, 1988, 399 (*tert-butyl ester, synth, ir, pmr, use*)
Ben Alloum, A. *et al*, *Synth. Commun.*, 1989, **19**, 2567 (*Et ester, synth, ir*)
Khare, A.B. *et al*, *Synthesis*, 1991, 405 (*Me ester, synth, ir, pmr, cmr, P-31 nmr*)
Moody, C.J. *et al*, *Tetrahedron*, 1992, **48**, 3991 (*Et ester, use*)

Diazo(dimethoxyphosphinyl) acetic acid D-1-00118

$(MeO)_2P(O)C(N_2)COOH$

$C_4H_7N_2O_5P$ M 194.0

Me ester: [60190-78-5]. *Trimethyl diazophosphonoacetate*
$C_5H_9N_2O_5P$ M 208.1 Yellow oil. $Bp_{0.002}$ 65-69°.

Nitrile: Diazo(dimethoxyphosphinyl) acetonitrile
$C_4H_6N_3O_3P$ M 175.0 Yellow oil. d_4^{20} 1.26. n_D^{20} 1.4710.

Khoklov, P.S. *et al*, *Zh. Obshch. Khim.*, 1984, **54**, 2641; *J. Gen. Chem. USSR (Engl. Transl.)*, 1984, **54**, 2359 (*nitrile*)
Khare, A.B. *et al*, *Synthesis*, 1991, 405 (*Me ester, ir, pmr, cmr, P-31 nmr*)

Diazoformylacetic acid D-1-00119

$OHCC(N_2)COOH$

$C_3H_2N_2O_3$ M 114.0

Et ester: [14762-48-2]. *Ethyl diazomalonaldehydate, 9CI*
$C_5H_6N_2O_3$ M 142.1 Used in synthesis of heterocycles. Yellow liq. $Bp_{0.7}$ 35-36°. n_D^{20} 1.4792.

Stojanovic, F.M. *et al*, *Coll. Czech. Chem. Comm.*, 1967, **32**, 2155 (*synth, uv*)
Connell, R.D. *et al*, *Tetrahedron*, 1993, **49**, 5445 (*synth, ir, pmr, cmr*)

(Diazomethylene) bisphosphonic acid, 9CI D-1-00120

Diazomethanebisphosphonic acid

$N_2C[P(O)(OH)_2]_2$

$CH_4N_2O_6P_2$ M 202.0

Tetra-Me ester: [54148-00-4]. *Tetramethyl (diazomethylene)bisphosphonate*
$C_5H_{12}N_2O_6P_2$ M 258.1 Cryst. (petrol).

Tetra-Et ester: [19734-17-9]. *Tetraethyl (diazomethylene)bisphosphonate*
$C_9H_{20}N_2O_6P_2$ M 314.2 Liq. $Bp_{0.3}$ 131-133°.

Regitz, M. *et al*, *Tet. Lett.*, 1968, 3171 (*tetra-Et ester*)
Khare, A.B. *et al*, *Synthesis*, 1991, 405 (*esters, synth, ir, pmr, cmr, P-31 nmr*)
Gross, H. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1993, **83**, 203 (*use*)
Cox, G.G. *et al*, *Tetrahedron*, 1994, **50**, 3195 (*use*)

P-(Diazomethylene) bis(phosphonous diamide), 9CI D-1-00121

$N_2{=}C[P(NH_2)_2]_2$

$CH_8N_6P_2$ M 166.0

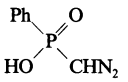
Octaisopropyl: [105309-80-6]. (*Diazomethylene)bis[phosphonous bis(diisopropylamide)*]. P-(*Diazomethylene*)-N,N,N′,N′,N″,N″,N‴,N‴-*octaisopropylbis(phosphonous diamide)*
$C_{25}H_{56}N_6P_2$ M 502.7 Air-stable orange cryst. ($MeCN/C_6H_6$). Mp 70-80° dec.

Octacyclohexyl: [141958-14-7]. P-(*Diazomethylene*)-N,N,N′,N′,N″,N″,N‴,N‴-*octacyclohexylbis(phosphonous diamide)*
$C_{49}H_{88}N_6P_2$ M 823.2 Orange cryst. (pentane at −20°). Mp 139-140°.

Baceiredo, A. *et al*, *J.A.C.S.*, 1986, **108**, 7868 (*synth, ir*)
Sicard, G. *et al*, *J.A.C.S.*, 1988, **110**, 2663 (*synth, reactions*)
Menu, M.J. *et al*, *J. Organomet. Chem.*, 1989, **372**, 201 (*synth, pmr, P-31 nmr, cryst struct*)
von Locquenghien, K.H. *et al*, *Chem. Comm.*, 1991, 1192 (*cmr, N-14 nmr*)
Réau, R. *et al*, *J.A.C.S.*, 1992, **114**, 6059 (*synth, ir, cmr, P-31 nmr*)

(Diazomethyl) phenylphosphinic acid D-1-00122

[89815-66-7]



$C_7H_7N_2O_2P$ M 182.1
Golden-yellow cryst. (as *tert*-butylammonium salt). Mp 157° dec. (*tert*-butylammonium salt). CAS no. refers to salt. Li salt also known.

Me ester: [56641-67-9].
$C_8H_9N_2O_2P$ M 196.1 Yellow oil.

Felcht, U. *et al*, *Chem. Ber.*, 1975, **108**, 2040 (*ester, synth, ir, uv, pmr*)
Hoffmann, K.-L. *et al*, *Chem. Ber.*, 1985, **118**, 3700 (*Li salt*)
Regitz, M. *et al*, *Tetrahedron*, 1985, **41**, 819 (*deriv, ir, pmr*)

P-(Diazomethyl)phosphonous diamide, 9CI, 8CI D-1-00123

$N_2CHP(NH_2)_2$

CH_5N_4P M 104.0

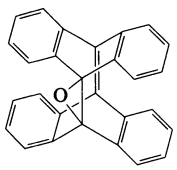
N,N,N′,N′-*Tetraisopropyl:* [97135-54-1]. P-(*Diazomethyl*)-N,N,N′,N′-*tetraisopropylphosphonous diamide*. (*Diazomethyl*)*phosphonous bis(diisopropylamide)*
$C_{13}H_{29}N_4P$ M 272.3 Red oil. Thermally unstable.

Baceiredo, A. *et al*, *J.A.C.S.*, 1985, **107**, 4781 (*tetraisopropyl, synth, ir, pmr, P-31 nmr, props*)
Baceiredo, A. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1986, **26**, 57 (*synth*)
Igau, A. *et al*, *J.A.C.S.*, 1988, **110**, 6463 (*tetraisopropyl, synth, ir, pmr, cmr, P-31 nmr*)
von Locquenghien, K.K. *et al*, *Chem. Comm.*, 1991, 1192 (*cmr, N-14 nmr*)
Sotiropoulos, J.M. *et al*, *Bull. Soc. Chim. Fr.*, 1992, **129**, 367 (*synth, ir, pmr, cmr, P-31 nmr*)

1*a*,6[1′,2′]:7,11*b*[1″,2″]-Dibenzenodibenzo[3,4:7,8]cyclooct[1,2-*b*]oxirene, 9CI D-1-00124

Tetradehydrodianthracene monoepoxide. 5,12:6,11-Di[1,2]benzenodibenzo[a,e] *cyclooctene monoepoxide*

[157528-69-3]



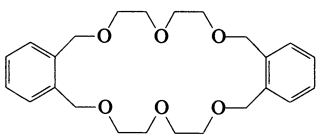
$C_{28}H_{16}O$ M 368.4
White or pale yellow powder. Mp 276° dec. Obt. *ca.* 80% pure.

Herges, R. *et al*, *Angew. Chem., Int. Ed.*, 1994, **33**, 993 (*synth, ir, pmr, cmr*)

Dibenzo-22-crown-6 D-1-00125

5,7,8,10,11,13,18,20,21,23,24,26-Dodecahydrodibenzo[i,t][*1,4,7,12,15,18*] *hexaoxacyclodocosin, 9CI*

[60985-77-5]

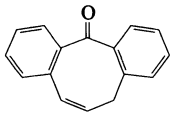


$C_{24}H_{32}O_6$ M 416.5
Cryst. (Me_2CO). Mp 85-86°.

Reinhoudt, D.N. *et al*, *Tetrahedron*, 1976, **32**, 1161 (*synth, pmr, cmr*)
Gray, R.T. *et al*, *J.C.S. Perkin 2*, 1977, 206 (*ms*)
Weber, E. *et al*, *Bull. Chem. Soc. Jpn.*, 1990, **63**, 3670 (*synth, ir, pmr*)
Ouchi, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1993, **66**, 2309 (*cryst struct*)

Dibenzo[*a,d*]cycloocten-12(5*H*)-one, 9CI D-1-00126

[149622-30-0]



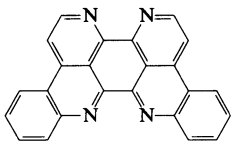
$C_{16}H_{12}O$ M 220.2
Oil.

Kobayashi, K. *et al, J.C.S. Perkin 1*, 1993, 825 (*synth, ir, pmr*)

Dibenzo[*b,j*]dipyrido[4,3,2-*de*:2′,3′,4′-*gh*][1,10]phenanthroline, 9CI D-1-00127

Eilatin

[120154-96-3]



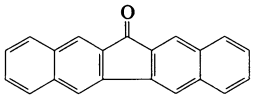
$C_{24}H_{12}N_4$ M 356.3
Alkaloid from the Red Sea tunicate *Eudistoma* sp. Bright yellow cryst. ($CHCl_3$/MeOH/H_2O). Mp >310°.

Rudi, A. *et al, Tet. Lett.*, 1988, **29**, 6655 (*uv, ir, pmr, cmr, ms, cryst struct*)
Rudi, A. *et al, J.O.C.*, 1989, **54**, 5331 (*isol, uv, ir, pmr, cmr, ms*)
Nakahara, S. *et al, Heterocycles*, 1993, **36**, 1139 (*synth*)
Gellerman, G. *et al, Tet. Lett.*, 1993, **34**, 1827 (*synth*)

12*H*-Dibenzo[*b,h*]fluoren-12-one, 9CI D-1-00128

2,3;6,7-Dibenzofluorenone

[53223-75-9]



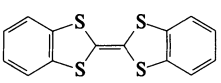
$C_{21}H_{12}O$ M 280.3
Bright yellow needles by subl., plates (C_6H_6). Mp 282.5-283.5° (275-276°).

Martin, R.H., *J.C.S.*, 1941, 679 (*synth*)
Morris, J.L. *et al, J.O.C.*, 1994, **59**, 6484 (*synth, pmr, ir*)

Dibenzotetrathiafulvalene D-1-00129

2-(1,3-Benzodithiol-2-ylidene)-1,3-benzodithiole, 9CI. DBTTF

[24648-13-3]



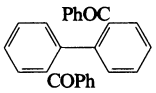
$C_{14}H_8S_4$ M 304.4
Electron donor for conducting charge-transfer salts. Yellow cryst. (C_6H_6). Mp 242.5-243° (235-237°).

Hurtley, W.R.H. *et al, J.C.S.*, 1926, 2263 (*synth*)
Hünig, S. *et al, Annalen*, 1973, 310 (*synth, uv*)
Nakayama, J. *et al, Bull. Chem. Soc. Jpn.*, 1976, **49**, 3567 (*synth*)
Emge, T.J. *et al, Mol. Cryst. Liq. Cryst.*, 1982, **87**, 137 (*cryst struct*)
Park, K.L. *et al, Magn. Reson. Chem.*, 1986, **24**, 831 (*pmr*)

2,2′-Dibenzoylbiphenyl D-1-00130

[*1,1′-Biphenyl*]-*2,2′-diylbis*[*phenylmethanone*], *9CI*

[24018-00-6]



$C_{26}H_{18}O_2$ M 362.4
Cryst. (EtOH or EtOH/Me_2CO). Mp 172-173° (165-168°).

Dioxime: [106569-09-9].
$C_{26}H_{20}N_2O_2$ M 392.4 Cryst. (Et_2O). Mp 185-186°.

Mono(ethylene ketal): [106568-95-0].
$C_{28}H_{22}O_3$ M 406.4 Cryst. (Et_2O). Mp 157-159°.

Bis(ethylene ketal): [106569-08-8].
$C_{30}H_{26}O_4$ M 450.5 Cryst. (Et_2O). Mp 147-149°.

Tschitschibabin, A.E. *et al, Ber.*, 1926, **59**, 654 (*synth*)
De Tar, D.F. *et al, J.A.C.S.*, 1950, **72**, 965 (*synth*)
Ames, D.E. *et al, Tetrahedron*, 1984, **40**, 1919 (*synth*)
Weitzberg, M. *et al, J.O.C.*, 1987, **52**, 529 (*deriv, synth, ir, pmr, ms*)

4,4′-Dibenzoylbiphenyl D-1-00131

[*1,1′-Biphenyl*]-*4,4′-diylbis*[*phenylmethanone*], *9CI*

[33090-29-8]

$C_{26}H_{18}O_2$ M 362.4
Mp 218°.

Dioxime:
$C_{26}H_{20}N_2O_2$ M 392.4 Cryst. (EtOH/Py). Mp 247°.

de Milt, C. *et al, J.A.C.S.*, 1940, **62**, 1952 (*synth, dioxime*)
Long, L.M. *et al, J.A.C.S.*, 1941, **63**, 1939 (*synth*)
Doesburg, H.M. *et al, Cryst. Struct. Commun.*, 1979, **8**, 377 (*cryst struct*)

Dibenzyl carbonate D-1-00132

Bis(phenylmethyl) carbonate, 9CI

[3459-92-5]

$PhCH_2OCOOCH_2Ph$

$C_{15}H_{14}O_3$ M 242.2
Selective benzylating reagent. Solid. Mp 27.3-29.1°. Bp_{12} 197-198°, $Bp_{1.1}$ 157°. n_D^{28} 1.5448.

Bowden, S.T., *J.C.S.*, 1939, 310 (*synth*)
Overberger, G.C. *et al, J.A.C.S.*, 1955, **77**, 4100 (*synth*)
Lissel, M. *et al, Chem. Ber.*, 1981, **114**, 1210 (*synth*)
Mizuno, T. *et al, Synthesis*, 1989, 636 (*synth, ir, pmr*)
Selva, M. *et al, J.C.S. Perkin 1*, 1995, 1889 (*synth, pmr, use*)

2,3-Dibenzyloxirane D-1-00133

2,3-Epoxy-1,4-diphenylbutene. 2,3-Bis(phenylmethyl)oxirane, 9CI

(1*RS*,2*RS*)-*form*

$C_{16}H_{16}O$ M 224.3

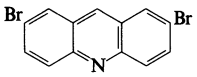
(1RS,2RS)-form [92695-14-2]
(±)-trans-*form*
Liq.

(1RS,2SR)-form [92695-13-1]
cis-*form*
Solid. Mp 31-33°.

Crotti, P. *et al, J.O.C.*, 1984, **49**, 4706 (*synth, pmr*)
Boehm, J.C. *et al, J. Med. Chem.*, 1993, **36**, 3333 (*synth, pmr*)

2,7-Dibromoacridine, 9CI D-1-00134

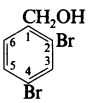
[1211-37-6]



$C_{13}H_7Br_2N$ M 337.0
Yellow leaflets. Mp 252°.

Acheson, R.M. *et al, J.C.S.*, 1954, 4142 (*synth*)
Kliegl, A. *et al, Chem. Ber.*, 1957, **90**, 60 (*synth*)
Budyka, M.F. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1989, **309**, 1126; *CA*, **112**, 178638h (*synth*)

2,4-Dibromobenzyl alcohol D-1-00135



$C_7H_6Br_2O$ M 265.9
Needles (CS_2). Mp 81-81.5°.

Olivier, S.C.J., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1926, **45**, 296 (*synth*)

2,5-Dibromobenzyl alcohol D-1-00136

2,5-Dibromobenzenemethanol, 9CI

[147034-01-3]

$C_7H_6Br_2O$ M 265.9
Cryst. (toluene). Mp 100.5-101°.

Shimura, Y. *et al, Synthesis*, 1993, 43 (*synth, ir, cmr, pmr*)

2,6-Dibromobenzyl alcohol D-1-00137

$C_7H_6Br_2O$ M 265.9
Needles (CS_2). Mp 110-110.5°.

Olivier, S.C.J., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1926, **45**, 296 (*synth*)

3,5-Dibromobenzyl alcohol D-1-00138

3,5-Dibromobenzenemethanol, 9CI

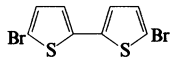
[145691-59-4]

$C_7H_6Br_2O$ M 265.9
Needles (CS_2 or H_2O). Mp 107-107.5°.

Olivier, S.C.J., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1926, **45**, 296 (*synth*)
Eur. Pat., 538 016, (1992); *CA*, **119**, 138977 (*synth*)

5,5′-Dibromo-2,2′-bithiophene, 9CI D-1-00139

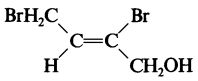
[4805-22-5]



$C_8H_4Br_2S_2$ M 324.0
Plates (Me_2CO); prisms (MeOH/THF). Mp 146° (143°).

Steinkopf, W. *et al*, *Annalen*, 1930, **482**, 251 (*synth*)
Kellogg, R.M. *et al*, *J.A.C.S.*, 1969, **34**, 343 (*synth, pmr*)
Fernando, Q. *et al*, *Acta Cryst. C*, 1988, **44**, 562 (*cryst struct*)
Zimmer, H. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1989, **46**, 153 (*synth, pmr, uv*)
Bäuerle, P. *et al*, *Synthesis*, 1993, 1099 (*synth pmr*)

2,4-Dibromo-2-buten-1-ol D-1-00140



$C_4H_6Br_2O$ M 229.8

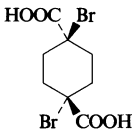
(Z)-form
Needles (hexane). Mp 39.2-40°.

Me ether: 2,4-Dibromo-1-methoxy-2-butene, 9CI
$C_5H_8Br_2O$ M 243.9 Oil. $Bp_{0.03}$ 70-80°.

[81447-08-7]

Seebach, D. *et al*, *Annalen*, 1994, 701 (*synth, cmr, pmr*)

1,4-Dibromo-1,4-cyclohexanedicarboxylic acid D-1-00141



$C_8H_{10}Br_2O_4$ M 329.9
Mp 304° dec.

(1RS,4RS)-form
trans-*form*

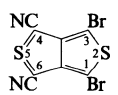
Dinitrile: 1,4-Dibromo-1,4-dicyanobenzene
$C_8H_8Br_2N_2$ M 291.9 Cryst. (C_6H_6). Mp 206°.

Barón, M. *et al*, *J. Mol. Struct.*, 1975, **24**, 432 (*synth*)
Echeverria, G. *et al*, *Acta Cryst. C*, 1995, **51**, 1023 (*cryst struct, dinitrile*)

1,3-Dibromo-4,6-dicyanothieno[3,4-*c*]thiophene D-1-00142

1,3-Dibromothieno[3,4-c]thiophene-5-S^{IV}-4,6-dicarbonitrile

[155632-47-6]



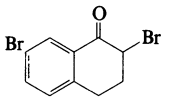
$C_8Br_2N_2S_2$ M 348.0
Dark purple cryst. Mp >360° dec. Stable in air.

Beye, N. *et al*, *J.O.C.*, 1994, **59**, 2223 (*synth, ir, cmr, uv, ms*)

2,7-Dibromo-3,4-dihydro-1(2*H*)-naphthalenone, 9CI D-1-00143

2,7-Dibromo-1-tetralone

[148378-71-6]



$C_{10}H_8Br_2O$ M 303.9
Brown cryst. Mp 76-77°.

Eur. Pat., 517 065, (1992); *CA*, **118**, 168890u (*synth, pmr*)

5,6-Dibromo-3,4-dihydro-1(2*H*)-naphthalenone D-1-00144

5,6-Dibromo-1-tetralone

$C_{10}H_8Br_2O$ M 303.9
Off-white solid. Mp 81-82°.

Combs, D.W. *et al*, *Synth. Commun.*, 1994, **24**, 2777 (*synth, pmr*)

5,7-Dibromo-3,4-dihydro-1(2*H*)-naphthalenone D-1-00145

5,7-Dibromo-1-tetralone

$C_{10}H_8Br_2O$ M 303.9
Light yellow prisms (hexane). Mp 60-61°.

Combs, D.W. *et al*, *Synth. Commun.*, 1994, **24**, 2777 (*synth, pmr*)

6,7-Dibromo-3,4-dihydro-1(2*H*)-naphthalenone D-1-00146

6,7-Dibromo-1-tetralone

$C_{10}H_8Br_2O$ M 303.9
Off-white solid. Mp 144-146°.

Combs, D.W. *et al*, *Synth. Commun.*, 1994, **24**, 2777 (*synth, pmr*)

2,2-Dibromoheptane D-1-00147

[156181-23-6]

$H_3C(CH_2)_4CBr_2CH_3$

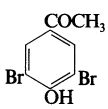
$C_7H_{14}Br_2$ M 257.9
Yellow liq. Bp_1 50-55°.

Kropp, P.J. *et al*, *J.O.C.*, 1994, **59**, 3102 (*synth, pmr, cmr*)

3,5-Dibromo-4-hydroxyacetophenone D-1-00148

4-Acetyl-2,6-dibromophenol

[2887-72-1]



$C_8H_6Br_2O_2$ M 293.9
Cryst. (C_6H_6). Mp 181-183°.

Phenylhydrazone: Mp 147°.

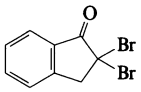
Me ether: 3′,5′-Dibromo-4′-methoxyacetophenone
$C_9H_8Br_2O_2$ M 307.9 Mp 78°.

Priestly, H.M. *et al*, *J.O.C.*, 1941, **5**, 358.

2,2-Dibromo-1-indanone D-1-00149

2,2-Dibromo-2,3-dihydro-1H-inden-1-one, 9CI

[7749-02-2]

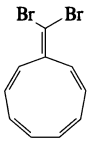


$C_9H_6Br_2O$ M 289.9
Cubes (EtOH). Mp 133-134°.

House, H.O. *et al*, *J.O.C.*, 1960, **82**, 1452 (*synth*)
Boger, D.L. *et al*, *J.O.C.*, 1994, **59**, 3453 (*synth, pmr, cmr, ir*)

9-(Dibromomethylene)-1,3,5,7-cyclononatetraene D-1-00150

10,10-Dibromononafulvene



$C_{10}H_8Br_2$ M 287.9
Pale yellow cryst. (Et_2O/pentane at −70°).

Chai, S. *et al*, *Helv. Chim. Acta*, 1994, **77**, 1377 (*synth, pmr, cmr*)

3-(Dibromomethylene)-1,4-pentadiyne, 9CI D-1-00151

3-(Dibromomethylidene)-1,4-pentadiyne

[133968-82-8]

$Br_2C{=}C(C{\equiv}CH)_2$

$C_6H_2Br_2$ M 233.8
Highly volatile cryst. Mp >35°.

Anthony, J. *et al*, *Helv. Chim. Acta*, 1995, **78**, 13.

1-(Dibromomethyl)-3-fluorobenzene, 9CI D-1-00152

α,α-*Dibromo*-m-*fluorotoluene*, *8CI*. m-*Fluorobenzal bromide*

[455-34-5]

$C_7H_5Br_2F$ M 267.9
Bp_8 108-110°. n_D^{25} 1.5847.

Varma, P.S. *et al*, *J. Indian Chem. Soc.*, 1944, **21**, 112 (*synth*)
Sheppard, W.A. *et al*, *Tetrahedron*, 1971, **27**, 945 (*nmr*)

1-(Dibromomethyl)-4-fluorobenzene, 9CI D-1-00153

α,α-*Dibromo*-p-*fluorotoluene*. p-*Fluorobenzal bromide*

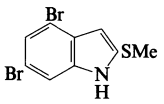
[6425-24-7]

$C_7H_5Br_2F$ M 267.9
$Bp_{2.4}$ 80°. n_D^{25} 1.5849.

Kerfanto, M. *et al*, *Bull. Soc. Chim. Fr.*, 1965, 3544.
Sheppard, W.A. *et al*, *Tetrahedron*, 1971, **27**, 945 (*synth, nmr*)

4,6-Dibromo-2-methylthio-1*H*-indole D-1-00154

[128351-88-2]



$C_9H_7Br_2NS$ M 321.0
Alkaloid from the Okinawan red alga *Laurencia brongniartii*. Cryst. (hexane/CCl_4). Mp 59-61°.

Tanaka, J. *et al*, *Tetrahedron*, 1989, **45**, 7301 (*isol, ir, pmr, ms, struct*)

4,4-Dibromooctane D-1-00155

[156181-22-5]

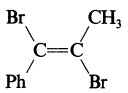
$H_3C(CH_2)_3CBr_2CH_2CH_2CH_3$

$C_8H_{16}Br_2$ M 272.0
Liq.

Kropp, P.J. *et al*, *J.O.C.*, 1994, **59**, 3102 (*synth, pmr, cmr*)

1,2-Dibromo-1-phenyl-1-propene D-1-00156

(*1,2-Dibromo-1-propenyl*)*benzene*, *9CI*

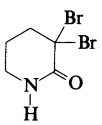


$C_9H_8Br_2$ M 275.9
(***E*-form** [67824-63-9]
Yellow liq.

Vemura, S. *et al*, *J.C.S. Perkin 1*, 1978, 1278 (*synth, pmr*)
Kropp, P.J. *et al*, *J.O.C.*, 1994, **59**, 3102 (*synth, pmr*)

3,3-Dibromo-2-piperidinone, 9CI D-1-00157

[26228-95-5]

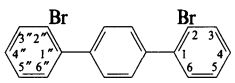


$C_5H_7Br_2NO$ M 256.9
Cryst. (EtOAc). Mp 177-179° (172-172°).

Uchikawa, O. *et al*, *J. Het. Chem.*, 1994, **31**, 1545.

2,2″-Dibromo-1,1′:4′,1″-terphenyl, 9CI D-1-00158

[95918-92-6]



$C_{18}H_{12}Br_2$ M 388.1
Needles (EtOH). Mp 137.5°.

Fujioka, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1984, **57**, 3494 (*synth*)

3,3″-Dibromo-1,1′:4′,1″-terphenyl, 9CI D-1-00159

[95918-94-8]

$C_{18}H_{12}Br_2$ M 388.1
Plates (C_6H_6). Mp 149.8°.

Fujioka, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1984, **47**, 3494 (*synth*)

4,4″-Dibromo-1,1′:4′,1″-terphenyl, 9CI D-1-00160

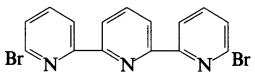
[17788-94-2]

$C_{18}H_{12}Br_2$ M 388.1
Prisms ($PhNO_2$). Mp 309-311°.

France, H. *et al*, *J.C.S.*, 1938, 1364 (*synth*)
Colonge, J. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 4370 (*synth, uv*)
Lapkin, I.I. *et al*, *Zh. Obshch. Khim.*, 1979, **49**, 167; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1979, **49**, 146 (*synth, uv*)

6,6″-Dibromo-2,2′:6′,2″-terpyridine, 9CI D-1-00161

[100366-66-3]

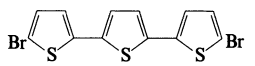


$C_{15}H_9Br_2N_3$ M 391.0
Needles or plates (toluene or $CHCl_3$). Mp 263-264° (248°).

Burstall, F.H., *J.C.S.*, 1938, 1662 (*synth*)
Newkome, G.R. *et al*, *J.O.C.*, 1986, **51**, 850 (*synth, pmr*)
Constable, E.C. *et al*, *J.C.S. Dalton*, 1987, 5 (*synth, ir, pmr, ms*)
Uchida, Y. *et al*, *Synthesis*, 1995, 939 (*synth, ms*)

5,5″-Dibromo-2,2′:5′,2″-terthiophene, 9CI D-1-00162

[98057-08-0]



$C_{12}H_6Br_2S_3$ M 406.1
Gold-yellow cryst. (MeOH/THF). Mp 159-160° (154-155°).

Morand, P. *et al*, *Tetrahedron*, 1988, **44**, 2403 (*synth, pmr, cmr, ms*)
Zimmer, H. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1989, **46**, 153 (*synth, ms*)
Bäuerle, P. *et al*, *Synthesis*, 1993, 1099 (*synth, pmr*)

1,1-Dibromo-3,3,3-trifluoropropene D-1-00163

$F_3CCH{=}CBr_2$

$C_3HBr_2F_3$ M 253.8
$Bp_{95\text{-}100}$ 41-55°.

Morken, P.A. *et al*, *J.A.C.S.*, 1993, **115**, 5430.

1,1-Dibromo-3,3,3-trifluoro-2-(trifluoromethyl)propene D-1-00164

1,1-Dibromo-2,2-bis(trifluoromethyl)ethylene

$(F_3C)_2C{=}CBr_2$

$C_4Br_2F_6$ M 321.8
Liq. Bp 56-61°, Bp 120-125°.

Morken, P.A. *et al*, *J.A.C.S.*, 1993, **115**, 5430.

Dibutoxymethane, 8CI D-1-00165

1,1′-[Methylenebis(oxy)]bisbutane, *9CI*. *Formaldehyde dibutyl acetal*. *Butylal*

[2568-90-3]

$H_2C(OCH_2CH_2CH_2CH_3)_2$

$C_9H_{20}O_2$ M 160.2
Liq. Bp_{12} 74-78°.

Fisher, C.L. *et al*, *J.A.C.S.*, 1989, **111**, 7379 (*synth, pmr*)
Wang, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1993, **66**, 2149 (*synth*)

Di-*tert*-butylamine D-1-00166

N-(*1,1-Dimethylethyl*)-*2-methyl-2-propanamine*, *9CI*

[21981-37-3]

$[(H_3C)_3C]_2NH$

$C_8H_{19}N$ M 129.2
Liq. Bp 119-120°.

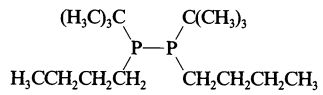
Hydrochloride: [63819-66-9].
Cryst. ($CHCl_3/Et_2O$). Mp 258-260° subl.

Kornblum, N. *et al*, *J.O.C.*, 1972, **37**, 2050 (*synth, pmr, ms*)
Kostyanovsky, R.G. *et al*, *Org. Mass Spectrom.*, 1972, **6**, 1199 (*ms*)
Back, T.G. *et al*, *J.C.S. Perkin 1*, 1977, 924 (*synth*)
Fjeldberg, T. *et al*, *J. Mol. Struct.*, 1986, **140**, 209 (*gas-phase struct*)
Schwartz, M.A. *et al*, *Tet. Lett.*, 1992, **33**, 1689 (*synth, pmr, cmr*)

1,2-Dibutyl-1,2-di-*tert*-butyldiphosphine D-1-00167

1,2-Dibutyl-1,2-bis(1,1-dimethylethyl) diphosphine

[82718-72-7]



$C_{16}H_{36}P_2$ M 290.4
Presumably stereoisomer mixt. Visc. liquid. $Bp_{0.5}$ 110-112°. n_D^{20} 1.5039.

Monoxide: [72170-78-6].
$C_{16}H_{36}OP_2$ M 306.4 Solid. Mp 107-110°. $Bp_{0.1}$ 118-123°.

Monosulfide: [82718-62-5].
$C_{16}H_{36}P_2S$ M 322.4 In equilib. (56%) with the tautomeric thioanhydride RR′-P-S-PRR′ (44%).

[74757-21-4, 74757-51-0]

Foss, V.L. *et al*, *Zh. Obshch. Khim.*, 1979, **49**, 1724; 1982, **52**, 1054, 1063; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1979, **49**, 1510; 1982, **52**, 916, 924 (*synth, derivs, props, P-31 nmr*)

1,1-Di-*tert*-butyl-2,2-dimethyldiphosphine D-1-00168

1,1-Bis(1,1-dimethylethyl)-2,2-dimethyldiphosphine, *9CI*

[57409-22-0]

$[(H_3C)_3C]_2PPMe_2$

$C_{10}H_{24}P_2$ M 206.2

Harris, R.K. *et al*, *J.C.S. Dalton*, 1979, 826 (*synth, P-31 nmr, struct*)
McFarlane, H.C.E. *et al*, *J.C.S. Dalton*, 1980, 240 (*pmr, P-31 nmr, struct*)
Ali, A.A.M. *et al*, *J.C.S. Dalton*, 1988, 2775 (*cmr, P-31 nmr*)

1,2-Di-*tert*-butyl-1,2-diphenyldiphosphine, 8CI D-1-00169

1,2-Bis(1,1-dimethylethyl)-1,2-diphenyldiphosphine, 9CI

[55793-26-5]

$(H_3C)_3CPPh—PPhC(CH_3)_3$

$C_{20}H_{28}P_2$ M 330.3
Presumable mixt. of stereoisomers. Solid. Mp 114°.

Monoxide: [72170-79-7].
$C_{20}H_{28}OP_2$ M 346.3 Solid. Mp 148-151°.

1,2-Dioxide: [18351-72-9].
$C_{20}H_{28}O_2P_2$ M 362.3 Cryst. (C_6H_6 or Me_2CO). Mp 228-229°.

[96254-44-3, 96254-45-4]

Brown, A.D. *et al*, *J.C.S.(C)*, 1968, 839 (*dioxide, pmr, ir*)
Schumann, H. *et al*, *J. Organomet. Chem.*, 1975, **88**, C13 (*synth, pmr, P-31 nmr*)
Dinritriev, V.I. *et al*, *Zh. Obshch. Khim.*, 1978, **48**, 1533; *J. Gen. Chem. USSR (Engl. Transl.)*, 1978, **48**, 1405 (*dioxide*)
Foss, V.L. *et al*, *Zh. Obshch. Khim.*, 1979, **49**, 1724; *J. Gen. Chem. USSR (Engl. Transl.)*, 1979, **49**, 1510 (*monoxide, synth, P-31 nmr*)

Dibutyl diselenide, 9CI D-1-00170

Butyl diselenide, 8CI

[20333-40-8]

$H_3C(CH_2)_3SeSe(CH_2)_3CH_3$

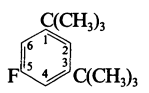
$C_8H_{18}Se_2$ M 272.1
Orange oil with offensive odour. Bp_{13} 129-130°. n_D^{20} 1.5402.

Backer, H.J. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1935, **54**, 531 (*synth*)
Stoner, G.G. *et al*, *J.A.C.S.*, 1948, **70**, 1113 (*synth*)
Bergson, G. *et al*, *Acta Chem. Scand.*, 1962, **16**, 1159 (*uv*)
Allum, K.G. *et al*, *Spectrochim. Acta A*, 1968, **24**, 927 (*ir, Raman*)
Agenäs, L.-B., *Ark. Kemi*, 1969, **30**, 497 (*ms*)
Sisler, H.H. *et al*, *J.O.C.*, 1971, **36**, 1700 (*synth*)
Anderson, J.A. *et al*, *Organometallics*, 1988, **7**, 267 (*cmr*)
Korchevin, N.A. *et al*, *Zh. Org. Khim.*, 1989, **59**, 1788; *J. Gen. Chem. USSR (Engl. Transl.)*, 1989, **59**, 1592 (*synth*)
Ping, L. *et al*, *Synth. Commun.*, 1993, **23**, 1721 (*synth, pmr*)

1,3-Di-*tert*-butyl-5-fluorobenzene D-1-00171

1,3-Bis(1,1-dimethylethyl)-5-fluorobenzene, 9CI

[38764-30-6]



$C_{14}H_{21}F$ M 208.3

Brownlee, R.T.C. *et al*, *J.A.C.S.*, 1972, **94**, 7208 (*F-19 nmr*)

2,4-Di-*tert*-butyl-1-fluorobenzene D-1-00172

2,4-Bis(1,1-dimethylethyl)-1-fluorobenzene

[65130-67-8]

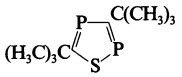
$C_{14}H_{21}F$ M 208.3
Oil. $Bp_{0.2}$ 55°.

Tashiro, M. *et al*, *Org. Prep. Proced. Int.*, 1977, **9**, 151 (*synth*)
Dehmlow, E.V. *et al*, *Tetrahedron*, 1995, **51**, 3755 (*synth, pmr*)

3,5-Di-*tert*-butyl-1,2,4-thiadiphosphole D-1-00173

3,5-Bis(1,1-dimethylethyl)-1,2,4-thiadiphosphole

[151961-31-8]



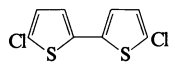
$C_{10}H_{18}P_2S$ M 232.2
Mp 10°.

Lindner, E. *et al*, *Angew. Chem., Int. Ed.*, 1993, **32**, 1424 (*synth, cmr, P-31 nmr*)
Lindner, E. *et al*, *J. Organomet. Chem.*, 1994, **464**, C31 (*synth, ms, P-31 nmr*)

5,5′-Dichloro-2,2′-bithiophene, 9CI D-1-00174

5,5′-Dichloro-2,2′-bithienyl

[18494-75-2]



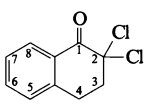
$C_8H_4Cl_2S_2$ M 235.1
Leaflets (EtOH). Mp 109°.

Uhlenbroek, J.H. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1960, **79**, 1181 (*synth*)
Veracini, C.A. *et al*, *J.C.S. Perkin 2*, 1973, 751 (*conformn, pmr*)
Abu-Eittah, R. *et al*, *Bull. Chem. Soc. Jpn.*, 1985, **58**, 2126 (*uv*)

2,2-Dichloro-3,4-dihydro-1(2*H*)-naphthalenone, 9CI D-1-00175

2,2-Dichloro-α-tetralone

[19221-36-4]



$C_{10}H_8Cl_2O$ M 215.0
Pale yellow cryst. (Et_2O/petrol). Mp 76°.

Stevens, C.L. *et al*, *J.A.C.S.*, 1955, **77**, 4590 (*synth*)
Nefedov, V.A., *Zh. Obshch. Khim.*, 1973, **43**, 2016; *J. Gen. Chem. USSR (Engl. Transl.)*, 1973, **43**, 2002 (*synth, ir*)
De Kimpe, N. *et al*, *Synth. Commun.*, 1978, **8**, 75 (*synth, pmr*)

5,6-Dichloro-3,4-dihydro-1(2*H*)-naphthalenone, 9CI D-1-00176

5,6-Dichloro-1-tetralone

[57915-84-1]

$C_{10}H_8Cl_2O$ M 215.0
Yellow cryst. (95% EtOH). Mp 89-92°.

Oxime: [153788-13-7].
$C_{10}H_9Cl_2NO$ M 230.0 Cryst. ($CHCl_3$). Mp 138-140°.

U.S. Pat., 3 919 316, (1975); *CA*, **84**, 43707n (*synth*)
Macchia, B. *et al*, *Eur. J. Med. Chem. (Chim. Ther.)*, 1993, **28**, 735 (*synth, pmr*)

6,7-Dichloro-3,4-dihydro-1(2*H*)-naphthalenone, 9CI D-1-00177

6,7-Dichloro-1-tetralone

[25095-57-2]

$C_{10}H_8Cl_2O$ M 215.0
Cryst. (EtOH aq.). Mp 106.5-107.5°.

Oxime: [34623-31-9].
$C_{10}H_9Cl_2NO$ M 230.0 Mp 204-205° (179-181°).

[34641-44-6]

Baker, B.R. *et al*, *J. Med. Chem.*, 1970, **13**, 87 (*synth*)
Rosowsky, A. *et al*, *J. Het. Chem.*, 1971, **8**, 809 (*synth, derivs, pmr*)
Owton, W.M. *et al*, *Synth. Commun.*, 1991, **21**, 981 (*synth, pmr*)
Macchia, B. *et al*, *Eur. J. Med. Chem. (Chim. Ther.)*, 1993, **28**, 735 (*synth, oxime*)

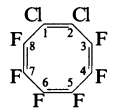
2,3-Dichloro-4-fluorobenzoic acid D-1-00178

$C_7H_3Cl_2FO_2$ M 209.0
Cryst. solid (heptane/Et_2O). Mp 189-191°.

Bennetau, B. *et al*, *J.C.S. Perkin 1*, 1995, 1265 (*synth, pmr, F-19 nmr*)

1,2-Dichloro-3,4,5,6,7,8-hexafluorocyclooctatetraene D-1-00179

[159190-52-0]



$C_8Cl_2F_6$ M 280.9
Cryst. by subl. Mp 35°. $Subl._{10}$ 33-34°.

Goldman, G.D. *et al*, *J.O.C.*, 1994, **59**, 7421 (*synth, ir, ms*)

1,8-Dichloro-2,3,4,5,6,7-hexafluorocyclooctatetraene D-1-00180

$C_8Cl_2F_6$ M 280.9
Liq.

Goldman, G.D. *et al*, *J.O.C.*, 1994, **59**, 7421 (*synth, ir, ms*)

1-(Dichloroiodo)-2,2,3,3,3-pentafluoropropane D-1-00181

$F_3CCF_2CH_2ICl_2$

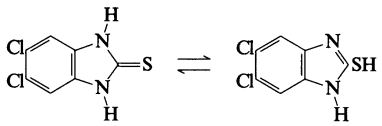
$C_3H_2Cl_2F_5I$ M 330.8
Pale yellow powder. Mp 70-71° dec.

Bravo, P. *et al*, *J.O.C.*, 1994, **59**, 6093 (*synth, pmr, F-19 nmr*)

5,6-Dichloro-2-mercaptobenzimidazole D-1-00182

5,6-Dichloro-1,3-dihydro-2H-benzimidazole-2-thione, 9CI. 5,6-Dichloro-2-benzimidazolethiol, 8CI. 5,6-Dichloro-2-benzimidazolethione

[19462-98-7]



$C_7H_4Cl_2N_2S$ M 219.0
Brown solid. Mp >360°.

Devivar, R.V. *et al, J. Med. Chem.*, 1994, **37**, 2942 (*synth, pmr, cmr, uv*)

2,6-Dichloro-3-methylbenzoic acid D-1-00183

$C_8H_6Cl_2O_2$ M 205.0
Cryst. solid (heptane/Et_2O). Mp 126-127°.

Bennetau, B. *et al, J.C.S. Perkin 1*, 1995, 1265 (*synth, pmr, cmr*)

1-(Dichloromethyl)-2-fluorobenzene, 9CI D-1-00184

α,α-Dichloro-o-fluorotoluene, 8CI. o-Fluorobenzal chloride

[320-65-0]

$C_7H_5Cl_2F$ M 179.0
d_4^{18} 1.31. Bp_{13} 71.6°. n_D^{19} 1.5225.

Schiemann, G. *et al, Ber., B*, 1937, **70**, 1416 (*synth*)
Ballester, M. *et al, J.A.C.S.*, 1964, **86**, 4276 (*uv*)

1-(Dichloromethyl)-3-fluorobenzene, 9CI D-1-00185

α,α-Dichloro-m-fluorotoluene, 8CI. m-Fluorobenzal chloride

[402-64-2]

$C_7H_5Cl_2F$ M 179.0
d_{16}^{16} 1.36. Bp 202-204°, Bp_6 77°. n_D^{25} 1.5238.

Schiemann, G., *Z. Phys. Chem. (Leipzig)*, 1931, **156**, 397.
Varma, P.S. *et al, J. Indian Chem. Soc.*, 1944, **21**, 112; *CA*, **39**, 1395 (*synth*)
Pelchowicz, Z. *et al, J.C.S.*, 1961, 5418 (*synth*)
Sheppard, W.A., *Tetrahedron*, 1971, **27**, 945 (*synth, nmr*)

1-(Dichloromethyl)-4-fluorobenzene, 9CI D-1-00186

α,α-Dichloro-p-fluorotoluene, 8CI. p-Fluorobenzal chloride

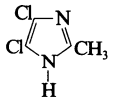
[456-19-9]

$C_7H_5Cl_2F$ M 179.0
Bp_{15} 81-83°, Bp_6 83°. n_D^{25} 1.5255.

Fukui, K. *et al, Nippon Kagaku Zasshi*, 1958, **79**, 1120.
Sheppard, W.A., *Tetrahedron*, 1971, **27**, 945 (*synth*)

4,5-Dichloro-2-methylimidazole, 9CI D-1-00187

[15965-33-0]

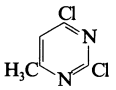


$C_4H_4Cl_2N_2$ M 150.9
Cryst. (H_2O). Mp 251-252° (247-248°).

Lutz, A.W. *et al, J. Het. Chem.*, 1967, **4**, 399 (*synth*)
Imbach, J.L. *et al, J. Het. Chem.*, 1967, **4**, 451 (*synth, pmr*)

2,4-Dichloro-6-methylpyrimidine, 9CI D-1-00188

[5424-21-5]



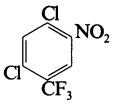
$C_5H_4Cl_2N_2$ M 163.0
Cryst. Mp 44-47°. Bp 219°.

Matswaka, T. *et al, Yakugaku Zasshi*, 1950, **70**, 134 (*synth*)
Brown, D.J. *et al, J.C.S.(B)*, 1971, 2214 (*pmr*)
Hung, J. *et al, J. Het. Chem.*, 1984, **21**, 741 (*synth*)

1,5-Dichloro-2-nitro-4-(trifluoromethyl)benzene, 9CI D-1-00189

2,4-Dichloro-5-nitrobenzotrifluoride. 2,4-Dichloro-α,α,α-trifluoro-5-nitrotoluene

[400-70-4]



$C_7H_2Cl_2F_3NO_2$ M 259.9
Mp 55-57°.

Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1381C.
Aldrich Library of NMR Spectra, 2nd edn., **1**, 1185C.
Fr. Pat., 745 293, (1933); *CA*, **27**, 4413 (*synth*)

4,4-Dichlorooctane D-1-00190

[156181-21-4]

$H_3C(CH_2)_3CCl_2CH_2CH_2CH_3$

$C_8H_{16}Cl_2$ M 183.1
Liq.

Kropp, P.J. *et al, J.O.C.*, 1994, **59**, 3102 (*synth, pmr*)

1,8-Dichloro-4-octyne D-1-00191

$ClCH_2CH_2CH_2C{\equiv}CCH_2CH_2CH_2Cl$

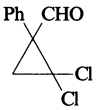
$C_8H_{12}Cl_2$ M 179.0
Liq.

Scott, L.T. *et al, J.A.C.S.*, 1994, **116**, 10275 (*synth, ir, pmr, cmr, ms*)

2,2-Dichloro-1-phenylcyclopropanecarboxaldehyde D-1-00192

1,1-Dichloro-2-formyl-2-phenylcyclopropane

[122801-51-8]



$C_{10}H_8Cl_2O$ M 215.0

(±)-*form*
$Bp_{1.2}$ 90-93°.

Di-Et acetal:
$C_{14}H_{18}Cl_2O_2$ M 289.2 Oil. $Bp_{1.0}$ 106-108°.

[85617-72-7]

Kagabu, S. *et al, J.C.S. Perkin 1*, 1994, 739.

Dichlorophosphonoacetic acid D-1-00193

[14112-51-7]

$(HO)_2P(O)CCl_2COOH$

$C_2H_3Cl_2O_5P$ M 208.9
Hygroscopic cryst. + $2H_2O$. V. sol. H_2O, EtOH, Me_2CO; insol. nonpolar solvs. Mp 85-125°.

Trichloride: Dichloro(dichlorophosphinyl) acetyl chloride
$C_2Cl_5O_2P$ M 264.2 Fuming liq. d_4^{20} 1.81. Bp_7 88-89°. n_D^{20} 1.5212.

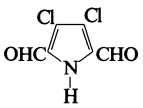
Trianilide: [14112-50-6]. *2,2-Dichloro-2-(dianilinophosphinyl)acetanilide*
$C_{20}H_{18}Cl_2N_3O_2P$ M 434.2 Cryst. (EtOH). Mp 153-155°.

Shevchenko, V.I. *et al, Zh. Obshch. Khim.*, 1966, **36**, 1645; *J. Gen. Chem. USSR (Engl. Transl.)*, 1966, **36**, 1645.

3,4-Dichloro-1*H*-pyrrole-2,5-dicarboxaldehyde D-1-00194

3,4-Dichloro-2,5-diformylpyrrole

[1196-68-5]

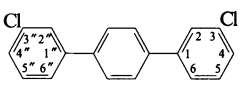


$C_6H_3Cl_2NO_2$ M 192.0
Cryst. (C_6H_6). Mp 185-186°. Previous refs. gave an incorrect M.p.

Cadamuro, S. *et al, J.C.S. Perkin 1*, 1993, 2939 (*synth, ir, pmr, cmr*)

3,3″-Dichloro-1,1′:4′,1″-terphenyl, 9CI D-1-00195

[159392-36-6]



$C_{18}H_{12}Cl_2$ M 299.1
Powder.

Musfeldt, J.L. *et al, J. Polym. Sci., Part B*, 1994, **32**, 2395 (*synth, pmr, cmr*)

4,4″-Dichloro-1,1′:4′,1″-terphenyl, 9CI D-1-00196

[21711-52-4]

$C_{18}H_{12}Cl_2$ M 299.1
Cryst. (EtOH). Mp 293°.

Bahurel, Y. *et al, Bull. Soc. Chim. Fr.*, 1968, 425S (*synth*)
Ger. Pat., 3 930 848, (1991); *CA*, **115**, 91816c (*synth*)

1,2-Dichloro-4-(trichloromethyl)benzene, 9CI D-1-00197

α,α,α-3,4-Pentachlorotoluene. 3,4-Dichlorobenzotrichloride

[13014-24-9]

$C_7H_3Cl_5$ M 264.3
Fp 25.8°. Bp 283.1°, Bp_{10} 140.1°.

Adv. Chem. Ser., 1955, **15**, 143 (***props***)
UK Pat., 771 416, (1957); *CA*, **51**, 16546h (*synth*)

1,3-Dichloro-2-(trichloromethyl)benzene D-1-00198

α,α,α-2,6-Pentachlorotoluene. 2,6-Dichlorobenzotrichloride

[54730-36-8]

$C_7H_3Cl_5$ M 264.3
Not purified.

Buchwald, P. *et al, Rev. Roum. Chim.*, 1974, **19**, 1221.

1,3-Dichloro-5-(trichloromethyl)benzene D-1-00199

α,α,α-3,5-Pentachlorotoluene. 3,5-Dichlorobenzotrichloride

$C_7H_3Cl_5$ M 264.3
Liq. Bp_3 124-126°.

Smith, W.T. *et al, J.O.C.*, 1961, **26**, 4713 (*synth*)

1,4-Dichloro-2-(trichloromethyl)benzene, 9CI D-1-00200

α,α,α-2,5-Pentachlorotoluene. 2,5-Dichlorobenzotrichloride

[10541-71-6]

$C_7H_3Cl_5$ M 264.3
Liq. Bp_{13} 150-160°.

Anspach, R. *et al, Annalen*, 1906, **346**, 322 (*synth*)
Sutherland, R.G. *et al, J. Organomet. Chem.*, 1991, **419**, 357 (*synth, pmr, cmr*)

2,4-Dichloro-1-(trichloromethyl)benzene, 9CI D-1-00201

α,α,α-2,4-Pentachlorotoluene, 8CI. 2,4-Dichlorobenzotrichloride

[13014-18-1]

$C_7H_3Cl_5$ M 264.3
Cryst. Mp 50°. Bp_{20} 155-159°.

Davies, W. *et al, Aust. J. Sci. Res., Ser. A*, 1952, **5**, 198 (*synth*)
Pews, R.G. *et al, Chem. Comm.*, 1978, 714 (*synth*)
Uspenskaya, I. *et al, Khim. Promst. (Moscow)*, 1980, 522; *CA*, **94**, 30272y (*synth*)

Dichloro(2,2,2-trifluoroethyl) iodine, 9CI D-1-00202

1-(Dichloroiodo)-2,2,2-trifluoroethane

[159763-01-6]

$F_3CCH_2ICl_2$

$C_2H_2Cl_2F_3I$ M 280.8
Yellow cryst. powder. Mp 108-111° dec.

Bravo, P. *et al, J.O.C.*, 1994, **59**, 6093 (*synth, pmr, F-19 nmr*)

1,2-Dichloro-4-(trifluoromethyl)benzene, 9CI D-1-00203

3,4-Dichloro-α,α,α-trifluorotoluene, 8CI. 3,4-Dichlorobenzotrifluoride

[328-84-7]

$C_7H_3Cl_2F_3$ M 215.0
Liq. d_4^{25} 1.4729. Bp 173-174°, Bp_{14} 63-65°. n_D^{25} 1.4719.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 919A.
Aldrich Library of NMR Spectra, 2nd edn., **1**, 807A.
Yagupolskii, L.M. *et al, Zh. Obshch. Khim.*, 1959, **29**, 2730; *J. Gen. Chem. USSR (Engl. Transl.)*, 1959, **29**, 2697 (*synth*)
Kogeyama, I. *et al, Kogyo Kagaku Zasshi*, 1962, **65**, 1203; *CA*, 1963, **58**, 5543 (*synth*)
Ushakov, A.A. *et al, Zh. Org. Khim.*, 1976, **12**, 158; *J. Org. Chem. USSR (Engl. Transl.)*, 1976, **12**, 153 (*synth, props*)

1,4-Dichloro-2-(trifluoromethyl)benzene, 9CI D-1-00204

2,5-Dichloro-α,α,α-trifluorotoluene, 8CI. 2,5-Dichlorobenzotrifluoride

[320-50-3]

$C_7H_3Cl_2F_3$ M 215.0
Liq. d_{20}^{20} 1.5009. Bp 174.6°, Bp_{16} 60°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 931C (*ir*)
Biedenkapp, D. *et al, J. Chem. Phys.*, 1968, **49**, 3933 (*Cl-35 nqr*)
Ushakov, A.A. *et al, Zh. Org. Khim.*, 1976, **12**, 158; *J. Org. Chem. USSR (Engl. Transl.)*, 1976, **12**, 153 (*synth, props*)
Freund, L. *et al, Makromol. Chem.*, 1989, **190**, 1561 (*synth, pmr, cmr, ms*)

2,4-Dichloro-1-(trifluoromethyl)benzene, 9CI D-1-00205

2,4-Dichloro-α,α,α-trifluorotoluene, 8CI. 2,4-Dichlorobenzotrifluoride

[320-60-5]

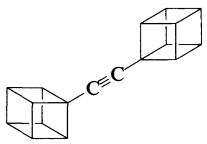
$C_7H_3Cl_2F_3$ M 215.0
Liq. Bp 117-118°. n_D^{20} 1.4788.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 931B.
Aldrich Library of NMR Spectra, 2nd edn., **1**, 804C.
Yurawecz, M.P. *et al, J. Assoc. Off. Anal. Chem.*, 1979, **62**, 36; 1981, **19**, 1123 (*glc, ms*)
U.S. Pat., 4 201 724, (1980); *CA*, **94**, 65296m (*synth*)

Dicubylacetylene D-1-00206

1,1′-(1,2-Ethynediyl) bispentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane, 9CI

[163332-96-5]



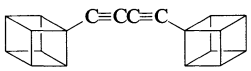
$C_{18}H_{14}$ M 230.3
Flat cryst. Mp >180° dec.

Eaton, P.E. *et al, J.A.C.S.*, 1994, **116**, 2588 (*synth, pmr, cmr, ms*)

1,4-Dicubyl-1,3-butadiyne D-1-00207

1,1′-(1,3-Butadiyne-1,4-diyl) bispentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane, 9CI

[163332-97-6]



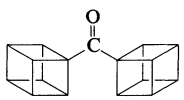
$C_{20}H_{14}$ M 254.3
Solid. Mp >140° dec.

Eaton, P.E. *et al, J.A.C.S.*, 1994, **116**, 2588 (*synth, pmr, cmr, ms, cryst struct*)

Dicubyl ketone D-1-00208

Bis(pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octyl) methanone, 9CI. Dicubylmethanone

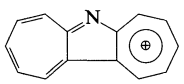
[163332-95-4]



$C_{17}H_{14}O$ M 234.2
Solid. Mp 175-177°.

Eaton, P.E. *et al, J.A.C.S.*, 1994, **116**, 7588 (*synth, pmr, cmr, ms*)

Dicyclohepta[*b,d*]pyrrolium(1+) D-1-00209

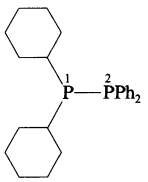


$C_{14}H_{10}N^{\oplus}$ M 192.2 (ion)

Tetrafluoroborate:
$C_{14}H_{10}BF_4N$ M 279.0 Greyish-green plates. Mp 160° dec.

Iino, Y. *et al, J.C.S. Perkin 1*, 1994, 2579 (*synth, uv*)

1,1-Dicyclohexyl-2,2-diphenyldiphosphine, 9CI, 8CI D-1-00210



$C_{24}H_{32}P_2$ M 382.4
Cryst. V. sol. Me_2CO, THF, CS_2, C_6H_6; sl. sol. Et_2O, petrol. Mp 92°.

1-Oxide: [61385-86-2].
$C_{24}H_{32}OP_2$ M 398.4 Solid. Mp 121-124°.

2-Oxide: [61385-83-9].
$C_{24}H_{32}OP_2$ M 398.4 Solid. Mp 160°.

1-Sulfide: [109012-12-6].
$C_{24}H_{32}P_2S$ M 414.5

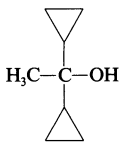
Disulfide: [3305-80-4].
$C_{24}H_{32}P_2S_2$ M 446.5 Cryst. (Me_2CO). V. sol. C_6H_6, CS_2; less sol. MeOH, Me_2CO. Mp 193-194°.

Isslieb, K. *et al*, *Chem. Ber.*, 1965, **98**, 1093 (*synth*)
Isslieb, K. *et al*, *J. Prakt. Chem.*, 1969, **311**, 463 (*synth*)
Foss, V.L. *et al*, *Zh. Obshch. Khim.*, 1976, **46**, 2382; 1979, **49**, 2418; *J. Gen. Chem. USSR (Engl. Transl.)*, 1976, **46**, 2280; 1979, **49**, 2134 (*synth, props*)

1,1-Dicyclopropylethanol D-1-00211

α-Cyclopropyl-α-methylcyclopropanemethanol, 9CI

[18895-50-6]



$C_8H_{14}O$ M 126.1
Liq. Bp_{10} 56.6-60°.

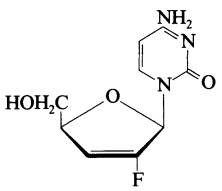
Me ether: 1,1-Dicyclopropyl-1-methoxyethane $C_9H_{16}O$ M 140.2 Pale yellow oil.

Hanack, M. *et al*, *Annalen*, 1963, **663**, 31 (*synth*)
Nishida, S. *et al*, *J. Organomet. Chem.*, 1978, **156**, 37 (*synth*)
Kelly, D.P. *et al*, *J.O.C.*, 1995, **60**, 1651 (*synth, ir, cmr*)

2′,3′-Didehydro-2′,3′-dideoxy-2′-fluorocytidine, 9CI D-1-00212

1-(2,3-Dideoxy-2-fluoro-β-D-glycero-2-pentenofuranosyl)cytosine

[122757-53-3]



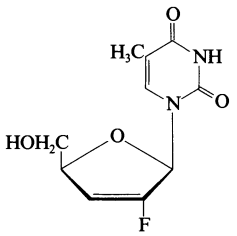
$C_9H_{10}FN_3O_3$ M 227.1
Cryst. (EtOAc). Mp 157-159°.

Martin, J.A. *et al*, *J. Med. Chem.*, 1990, **33**, 2137 (*synth, pmr*)
Sterzycki, R.Z. *et al*, *J. Med. Chem.*, 1990, **33**, 2150 (*synth, pmr, ms*)

2′,3′-Didehydro-2′,3′-dideoxy-2′-fluorothymidine D-1-00213

2′,3′-Didehydro-2′,3′-dideoxy-2′-fluoro-5-methyluridine, 9CI

[122757-54-4]

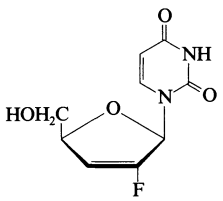


$C_{10}H_{11}FN_2O_4$ M 242.2
Cryst. (EtOAc). Mp 152-154°.

Martin, J.A. *et al*, *J. Med. Chem.*, 1990, **33**, 2137 (*synth, pmr*)

2′,3′-Didehydro-2′,3′-dideoxy-2′-fluorouridine D-1-00214

[122757-52-2]

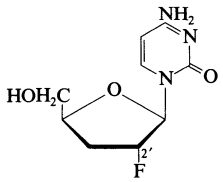


$C_9H_9FN_2O_4$ M 228.1
Cryst. (EtOAc/hexane). Mp 162-163°.

Martin, J.A. *et al*, *J. Med. Chem.*, 1990, **33**, 2137 (*synth, pmr*)

2′,3′-Dideoxy-2′-fluorocytidine, 9CI D-1-00215

4-Amino-1-(2,3-dideoxy-2-fluoro-β-D-erythro-pentofuranosyl)-2(1H)-pyrimidinone, 9CI. 1-(2,3-Dideoxy-2-fluoro-β-D-erythro-pentofuranosyl)cytosine



$C_9H_{12}FN_3O_3$ M 229.2
Cryst. (EtOH) (as hydrochloride). Mp 219-220°.

2′-Epimer: [119555-47-4]. *F-DDC*
$C_9H_{12}FN_3O_3$ M 229.2 Shows activity against HIV. Cryst. (EtOH). Mp 205-208°. $[\alpha]_{365}$ +710.15 (c, 1.027 in H_2O), $[\alpha]_D^{20}$ +168.7 (c, 0.5 in H_2O).

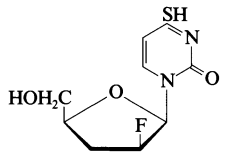
2′-Epimer, di-Ac: [128115-08-2].
$C_{13}H_{16}FN_3O_5$ M 313.2 Cryst. (MeOH). Mp 223-224°.

Martin, J.A. *et al*, *J. Med. Chem.*, 1990, **33**, 2137 (*synth, pmr, ms*)
Watanabe, K.A. *et al*, *J. Med. Chem.*, 1990, **33**, 2145 (*synth, pmr*)
Sterzycki, R.Z. *et al*, *J. Med. Chem.*, 1990, **33**, 2150 (*synth, pmr, cmr, uv, ir*)
Okabe, M. *et al*, *J.O.C.*, 1991, **56**, 4392 (*synth, pmr, ir*)

1-(2,3-Dideoxy-2-fluoro-β-D-*threo*-pentofuranosyl)-4-thiouracil D-1-00216

1-(2,3-Dideoxy-2-fluoro-β-D-threo-pentofuranosyl)-3,4-dihydro-4-thioxo-2(1H)-pyrimidinone, 9CI

[128632-07-5]



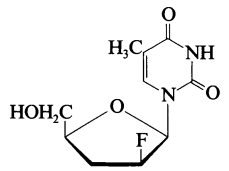
$C_9H_{11}FN_2O_3S$ M 246.2
Cryst. ($EtOH/Et_2O$). Mp 134-137°.

Sterzycki, R.Z. *et al*, *J. Med. Chem.*, 1990, **33**, 2150 (*synth, pmr, cmr, ms*)

1-(2,3-Dideoxy-2-fluoro-β-D-*threo*-pentofuranosyl) thymine D-1-00217

1-(2,3-Dideoxy-2-fluoro-β-D-threo-pentofuranosyl)-5-methyl-2,4(1H,3H)-pyrimidinedione, 9CI

[121353-89-7]



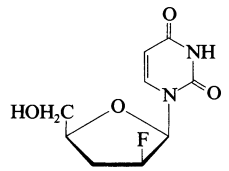
$C_{10}H_{13}FN_2O_4$ M 244.2
Cryst. (CH_2Cl_2/Et_2O/hexane). Mp 162-164°.

Sterzycki, R.Z. *et al*, *J. Med. Chem.*, 1990, **33**, 2150 (*synth, pmr, cmr, ms*)

1-(2,3-Dideoxy-2-fluoro-β-D-*threo*-pentofuranosyl)uracil D-1-00218

1-(2,3-Dideoxy-2-fluoro-β-D-threo-pentofuranosyl)-2,4(1H,3H)-pyrimidinedione, 9CI

[124424-25-5]

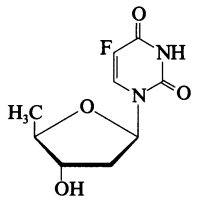


$C_9H_{11}FN_2O_4$ M 230.1
Cryst. Mp 159-162°.

Sterzycki, R.Z. *et al*, *J. Med. Chem.*, 1990, **33**, 2150 (*synth, pmr, cmr*)

2′,5′-Dideoxy-5-fluorouridine D-1-00219

[61168-97-6]

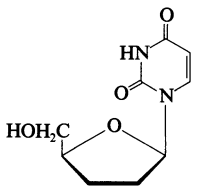


$C_9H_{11}FN_2O_4$ M 230.1
Cryst. (EtOH). Mp 171-173° (168°).

Cook, A.F. *et al*, *J. Med. Chem.*, 1980, **23**, 852 (*synth, pmr, uv*)
Chae, W.-G. *et al*, *J.O.C.*, 1992, **57**, 1002 (*synth, pmr, F-19 nmr*)

2′,3′-Dideoxyuridine, 9CI D-1-00220

[5983-09-5]



$C_9H_{12}N_2O_4$ M 212.2
Used in antiviral and anticancer studies. Cryst. Mp 127-129°. $[\alpha]_D^{20}$ +34 (c, 0.4 in H_2O).

5′-Ac: [102935-28-4].
$C_{11}H_{14}N_2O_5$ M 254.2 Cryst. Mp 80.1-80.6°.

5′-Benzoyl: [28616-91-3].
$C_{16}H_{16}N_2O_5$ M 316.3 Needles (EtOAc). Mp 143-144°.

Pfitzner, K.E. *et al*, *J.O.C.*, 1964, **29**, 1508 (*synth*)
Furukawa, Y. *et al*, *Chem. Pharm. Bull.*, 1970, **18**, 554 (*synth, benzoyl, uv, pmr*)
Shiragami, H. *et al*, *J.O.C.*, 1988, **53**, 5170 (*synth, Ac, uv, pmr*)
Jung, M.E. *et al*, *Tet. Lett.*, 1992, **33**, 2921 (*synth, benzoyl*)

Didodecyldimethylammonium(1+), 8CI D-1-00221

N-*Dodecyl*-N,N-*dimethyl-1-dodecanaminium, 9CI*

$[H_3C(CH_2)_{11}]_2N^{\oplus}Me_2$

$C_{26}H_{56}N^{\oplus}$ M 382.7 (ion)
Chloride: [3401-74-9].
$C_{26}H_{56}ClN$ M 418.1 Cryst. (Et_2O/EtOAc). Mp 130-131°.
Bromide: [3282-73-3].
$C_{26}H_{56}BrN$ M 462.6 Cryst. (EtOAc). Mp 169-171°.

Cipiciani, A. *et al*, *J.C.S. Perkin 2*, 1987, 541 (*synth*)

Didodecylphosphine D-1-00222

[13176-24-4]

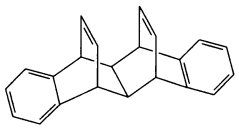
$[H_3C(CH_2)_{11}]_2PH$

$C_{24}H_{51}P$ M 370.6
Liq. $Bp_{0.022}$ 188-195°.

Hays, H.R., *J.O.C.*, 1966, **31**, 3817.

5,12:6,11-Dietheno-5,5*a*,6,11,11*a*,12-hexahydronaphthacene D-1-00223

4,5:9,10-Bisbenzotetracyclo[6.2.2.2^{3,6}.0^{2,7}]tetradeca-4,9,11,13-tetraene



$C_{22}H_{18}$ M 282.3
Cryst. (Et_2O/hexane). Mp 204-205°.

Lin, C.T. *et al*, *Tetrahedron*, 1995, **51**, 2907 (*synth, ir, pmr, cmr, ms, cryst struct, props*)

(Diethoxyphosphino)acetic acid D-1-00224

$(EtO)_2PCH_2COOH$

$C_6H_{13}O_4P$ M 180.1
Me ester: [688-44-8].
Methyl(diethoxyphosphino)acetate
$C_7H_{15}O_4P$ M 194.1 Liq. d_4^{20} 1.07. Bp_8 84-85°. n_D^{20} 1.4420.
Et ester: [688-49-3]. *Ethyl(diethoxyphosphino) acetate*
$C_8H_{17}O_4P$ M 208.1 Liq. d_4^{20} 1.03. Bp_9 95-96°. n_D^{20} 1.4380.

Proskurnina, M.V. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **159**, 619; *CA*, **62**, 6508 (*Me ester*)
Novikova, Z. *et al*, *Zh. Obshch. Khim.*, 1969, **39**, 1060 (*synth, ir, pmr*)
Cao, Y. *et al*, *Aust. J. Chem.*, 1994, **47**, 903 (*Me ester, synth, pmr, cmr*)

1,1-Diethyl-2,2-diphenyldiphosphine, 9CI D-1-00225

[3040-62-8]

Et_2PPPh_2

$C_{16}H_{20}P_2$ M 274.2
[3305-81-5]

Harris, R.K. *et al*, *J.C.S. Dalton*, 1979, 826 (*synth, cmr, P-31 nmr*)

1,2-Diethyl-1,2-diphenyldiphosphine D-1-00226

[3619-93-0]

PhPEt—PEtPh

$C_{16}H_{20}P_2$ M 274.2
Prep. as stereoisomeric mixt. Solid. Mp 48-50°. Bp_2 160-164°, $Bp_{0.01}$ 125°.
[26978-40-5]

Issleib, K. *et al*, *Chem. Ber.*, 1966, **99**, 1310 (*synth*)
Issleib, K. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **385**, 47; 1977, **437**, 5 (*synth, P-31 nmr*)
Appel, R. *et al*, *Chem. Ber.*, 1977, **110**, 376 (*synth, P-31 nmr*)
Horner, L. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1980, **8**, 235 (*synth*)

2,2-Diethyl-4-pentenoic acid, 9CI D-1-00227

Diethylallylacetic acid

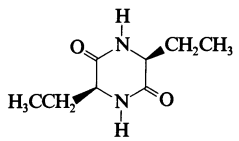
[67020-02-4]

$H_2C{=}CHCH_2C(CH_2CH_3)_2COOH$

$C_9H_{16}O_2$ M 156.2
Amide: [512-48-1]. *Diethylallylacetamide. **Valdetamide, INN.** Epinoval. Novonal. DAPA*
$C_9H_{17}NO$ M 155.2 Mild hypnotic. Mp 75-76°.
▶ LD_{50} (hmn, orl) 300 mg/kg. LD_{50} (rat, orl) 400 mg/kg. SB2145000.

Bockmühl, M. *et al*, *Dtsch. Med. Wochenschr.*, 1928, **54**, 270, 271 (*amide*)
Beyer, K.H., *Dtsch. Apoth. -Ztg.*, 1978, **118**, 1303 (*rev, amide*)
Klug, E. *et al*, *Arzneim.-Forsch.*, 1979, **29**, 1651 (*anal, metab, amide*)
Eur. Pat., 33 233, (1981) (*Sterwin*); *CA*, **95**, 203337 (*synth*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DJU200.

3,6-Diethyl-2,5-piperazinedione D-1-00228



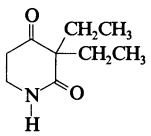
$C_8H_{14}N_2O_2$ M 170.2
(2S,5S)-form
Intermed. for assym. synth. of α,α-disubt. amino acids. Cryst. flakes. Mp 258-260°.

Liu, W. *et al*, *J.C.S. Perkin 1*, 1995, 553 (*synth, pmr, cmr, use*)

3,3-Diethyl-2,4-piperidinedione, 9CI D-1-00229

Piperidione. Ascron. Dihyprylone. Sedilan. Sedulon. Tusseval. Nu 1510

[77-03-2]



$C_9H_{15}NO_2$ M 169.2
Sedative. Antitussive. Needles (hot H_2O). Mp 103-105°.
▶ LD_{Lo} (rat, orl) 1100 mg/kg. TM7345500.

Tsukita, K. *et al*, *Yakugaku Zasshi*, 1949, **69**, 194; *CA*, **44**, 1506h (*synth*)
Kohei, I., *CA*, 1959, **53**, 20580e (*pharmacol*)
Bernard, K. *et al*, *CA*, 1959, **53**, 7408f (*metab*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 751.

1,1-Diethyl-2-(trifluoromethyl) diphosphine D-1-00230

[117583-76-3]

$Et_2P—PHCF_3$

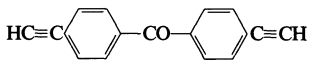
$C_5H_{11}F_3P_2$ M 190.0

Avens, L.R. *et al*, *Inorg. Chem.*, 1989, **28**, 200, 205 (*synth, F-19 nmr, P-31 nmr*)

4,4′-Diethynylbenzophenone D-1-00231

Bis(4-ethynylphenyl)methanone

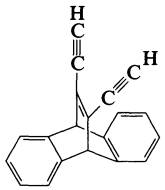
[147613-78-3]



$C_{17}H_{10}O$ M 230.2
Mp 154-155°.

Royles, B.J.L. *et al*, *J.C.S. Perkin 1*, 1994, 355 (*synth*)

11,12-Diethynyl-9,10-dihydro-9,10-ethenoanthracene D-1-00232



$C_{20}H_{12}$ M 252.3
Unstable cryst.

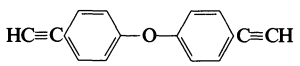
▶ Has exploded.

Diederich, F. *et al*, *Helv. Chim. Acta*, 1994, **77**, 1441 (*synth, pmr, cmr*)

4,4′-Diethynyldiphenyl ether D-1-00233

1,1′-Oxybis[4-ethynylbenzene]

[21368-80-9]



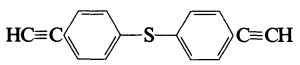
$C_{16}H_{10}O$ M 218.2
Mp 77-77.5° (72°).

Royles, B.J.L. *et al*, *J.C.S. Perkin 1*, 1994, 355.

4,4′-Diethynyldiphenyl sulfide D-1-00234

1,1′-Thiobis[4-ethynylbenzene]

[27594-21-4]



$C_{16}H_{10}S$ M 234.3
Mp 117-120° (114-116°).

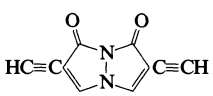
S,S-*Dioxide: 4,4′-Diethynyldiphenyl sulfone*
$C_{16}H_{10}O_2S$ M 266.3 Mp 177-178.5° (160°).

Royles, B.J.L. *et al*, *J.C.S. Perkin 1*, 1994, 355.

2,6-Diethynyl-1*H*,7*H*-pyrazolo[1,2-*a*]pyrazole-1,7-dione, 9CI D-1-00235

syn-(*Hydro,ethynyl)binane. 3,7-Diethynyl-1,5-diazabicyclo[3.3.0]octa-3,6-diene-2,8-dione*

[153498-38-5]

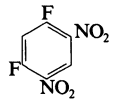


$C_{10}H_4N_2O_2$ M 184.1
Red-orange cryst. Fluoresces strongly in MeCN soln.

Kosower, E.M. *et al*, *Chem. Comm.*, 1993, 1644 (*synth, ir, pmr, cryst struct, uv*)

1,5-Difluoro-2,4-dinitrobenzene, 9CI D-1-00236

[327-92-4]

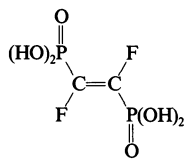


$C_6H_2F_2N_2O_4$ M 204.0
Protein cross-linking agent. Cryst. Mp 74-75°. Bp_2 132°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1217A.
Aldrich Library of NMR Spectra, 2nd edn., **1**, 1183A.
Swarts, F., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1915, **35**, 154 (*synth*)
Ger. Pat., 1 018 042, (1953); *CA*, **53**, 17054f (*synth*)
U.S. Pat., 2 891 074, (1954); *CA*, **53**, 16057g (*synth*)
Marley, P. *et al*, *Carlsberg Res. Commun.*, 1984, **49**, 591; *CA*, **102**, 167132f (*use*)
Eur. Pat., 246 809, (1987); *CA*, **108**, 62501w (*use*)

1,2-Difluoro-1,2-ethylenediphosphonic acid D-1-00237

(1,2-Difluoro-1,2-ethenediyl)bisphosphonic acid



(*E*)-*form*

$C_2H_4F_2O_6P_2$ M 223.9
Syrup (mixt. of geom. isomers).

(*E*)-*form* [126295-81-6]

Tetra-Et ether: [120932-35-6].
$C_{10}H_{20}F_2O_6P_2$ M 336.2 Liq. Bp_1 180-186°.

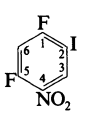
Tetrakis(trimethylsilyl) ester: [130335-55-6].
Tetrakis(trimethylsilyl) (1,2-difluoro-1,2-ethanediyl)bisphosphonate
$C_{14}H_{36}F_2O_6P_2Si_4$ M 512.7 Viscous liq.

[120932-34-5, 130312-53-7, 130312-54-8]

Dittrich, R. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1981, **10**, 127 (*ester, synth, F-19 nmr*)
Kadyrov, A.A. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1988, 1855; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1988, 1686 (*synth, pmr, ms*)
Sprague, L.G. *et al*, *J. Fluorine Chem.*, 1990, **49**, 75 (*ester, synth, ir, F-19 nmr, P-31 nmr*)
Su, D. *et al*, *J.A.C.S.*, 1990, **112**, 3152 (*synth, ms, pmr, F-19 nmr, P-31 nmr*)

1,5-Difluoro-2-iodo-4-nitrobenzene D-1-00238

[148388-74-3]



$C_6H_2F_2INO_2$ M 284.9
Liq. $Bp_{0.1}$ 65-67°.

Olah, G.A. *et al*, *J.O.C.*, 1993, **58**, 3194 (*synth, cmr, ms*)

2,4-Difluoro-3-mercaptobenzoic acid D-1-00239

$C_7H_4F_2O_2S$ M 190.1

S-*Me:*
$C_8H_6F_2O_2S$ M 204.1 Cryst. solid (heptane/Et_2O). Mp 169-171°.

Bennetau, B. *et al*, *J.C.S. Perkin 1*, 1995, 1265 (*synth, pmr, cmr*)

3,4-Difluoro-2-mercaptobenzoic acid D-1-00240

$C_7H_4F_2O_2S$ M 190.1

S-*Me:*
$C_8H_6F_2O_2S$ M 204.1 Cryst. solid (heptane/Et_2O). Mp 149-150°.

Bennetau, B. *et al*, *J.C.S. Perkin 1*, 1995, 1265 (*synth, pmr, cmr, F-19 nmr*)

(Difluoromethyl) diphenylphosphine D-1-00241

Ph_2PCHF_2

$C_{13}H_{11}F_2P$ M 236.2

Oxide: [129932-29-2].
$C_{13}H_{11}F_2OP$ M 252.2 Wittig-Horner reagent for synth. of 1,1-difluoroalkenes. Solid. Mp 93-94°.

Edwards, M.L. *et al*, *Tet. Lett.*, 1990, **31**, 5571 (*synth, ir, pmr, F-19 nmr, use*)

(Difluoromethyl)phenyl selenide D-1-00242

[(*Difluoromethyl)seleno]benzene, 9CI*

[101220-61-5]

$F_2CHSePh$

$C_7H_6F_2Se$ M 207.0
Oil. Bp_{35} 89-90°, Bp_9 63-64°.

Se-*Oxide:* [147912-92-3]. [(*Difluoromethyl) seleninyl]benzene, 9CI*
$C_7H_6F_2OSe$ M 223.0 Cryst. (hexane). Mp 97-98°.

Suzuki, H. *et al*, *Synthesis*, 1985, 497 (*synth, ir, pmr*)
Uneyama, K. *et al*, *J.O.C.*, 1995, **60**, 370 (*synth, ir, pmr, cmr, F-19 nmr*)

(Difluoromethyl) phenyl telluride D-1-00243

[101220-66-0]

$F_2CHTePh$

$C_7H_6F_2Te$ M 255.7
Oil. Bp_{19} 100-101°.

Suzuki, H. *et al*, *Synthesis*, 1985, 497 (*synth, ir, pmr*)

[1,2-Difluoro-2-(pentafluoro-λ⁶-sulfonyl)ethenyl] phosphonic acid D-1-00244

(2-Phosphono-1,2-difluoroethenyl) pentafluorosulfur

$F_5SCF{=}CFP(O)(OH)_2$

$C_2H_2F_7O_3PS$ M 270.0

Di-Et ester: [*2-(Diethoxyphosphinyl)-1,2-difluoroethenyl]pentafluorosulfur, 9CI*
$C_6H_{10}F_7O_3PS$ M 326.1 Liq. $Bp_{0.04}$ 38°, $Bp_{0.001}$ 37°. Approx. 1:1 (*E*)/(*Z*) composition.

Bis(trimethylsilyl) ester: [*2-Bis(trimethylsilyloxyphosphinyl)-1,2-difluoroethenyl]pentafluorosulfur, 9CI*
$C_8H_{18}F_7O_3PSSi_2$ M 414.4 Liq. $Bp_{0.1}$ 72°, $Bp_{0.001}$ 38°. Approx. 1:1 (*E*)/(*Z*) composition.

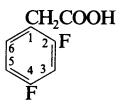
[133640-79-6, 133640-80-9]

Wessolowski, H. *et al, Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **60**, 201 (*synth, ms, ir, F-19 nmr, P-31 nmr*)
Wessolowski, H. *et al, Z. Naturforsch., B*, 1991, **46**, 126 (*synth, ms, ir, F-19 nmr, P-31 nmr*)

2,4-Difluorophenylacetic acid D-1-00245

2,4-Difluorobenzeneacetic acid, 9CI

[81228-09-3]



$C_8H_6F_2O_2$ M 172.1
Mp 117-119°.

Nitrile: [656-35-9].
$C_8H_5F_2N$ M 153.1 d 1.25. Bp_{10} 98°.

[95299-17-5, 129409-54-7]

Jerumanis, S. *et al, Bull. Soc. Chim. Belg.*, 1960, **69**, 312 (*nitrile*)
Eur. Pat., 41 233, (1981); *CA*, **96**, 142442 (*synth*)
Ger. Pat., 3 314 249, (1984); *CA*, **102**, 113053 (*synth, ester*)
Mattiello, L. *et al, J.C.S. Perkin 2*, 1990, 1041 (*ester, pmr*)

2,6-Difluorophenylacetic acid D-1-00246

2,6-Difluorobenzeneacetic acid

[85068-28-6]

$C_8H_6F_2O_2$ M 172.1
Mp 100-102°.

Nitrile: [654-01-3].
$C_8H_5F_2N$ M 153.1 d 1.24. Bp_{27} 109°.

Jerumanis, S. *et al, Bull. Soc. Chim. Belg.*, 1960, **69**, 312.

3,4-Difluorophenylacetic acid D-1-00247

3,4-Difluorobenzeneacetic acid

[658-93-5]

$C_8H_6F_2O_2$ M 172.1
Cryst. (hexane). Mp 46-50° (40-42°).

Nitrile: [658-99-1].
$C_8H_5F_2N$ M 153.1 d 1.24. Bp_{13} 110-120°.

[129409-55-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1405A.
Baltzly, R. *et al, J.O.C.*, 1961, **26**, 2353 (*synth*)

Difluorophenylacetic acid D-1-00248

α,α-Difluorobenzeneacetic acid

[360-03-2]

$PhCF_2COOH$

$C_8H_6F_2O_2$ M 172.1
Cryst. ($CFCl_3$ or petrol). Mp 76-77° (62-63°).

Me ester: [56071-96-6].
$C_9H_8F_2O_2$ M 186.1 Bp_{20} 100-101°.

Chloride:
$C_8H_5ClF_2O$ M 190.5 Bp_{15} 67-68°.

Amide: [383-19-7].
$C_8H_7F_2NO$ M 171.1 Cryst. (C_6H_6 or H_2O). Mp 114-115°.

Nitrile: [2002-72-4]. *α,α-Difluorobenzeneacetonitrile. Cyanodifluorophenylmethane. α-Cyano-α,α-difluorotoluene*
$C_8H_5F_2N$ M 153.1 Liq. Bp_{98} 94-95°.

[2248-46-6]

Middleton, W.J. *et al, J.O.C.*, 1980, **45**, 2883 (*synth*)
Taguchi, T. *et al, Tet. Lett.*, 1986, **27**, 6103 (*synth, ester*)

1,3-Difluoropropane D-1-00249

[462-39-5]

$FCH_2CH_2CH_2F$

$C_3H_6F_2$ M 80.0
d_4^{25} 1.00. Bp 40-42°. n_D^{26} 1.3190.

Hoffman, F.W., *J.O.C.*, 1949, **14**, 105.

2,2-Difluoropropane D-1-00250

[420-45-1]

$H_3CCF_2CH_3$

$C_3H_6F_2$ M 80.0
Formerly used as aerosol propellant. Bp −1°.

Austin, P.R. *et al, J.A.C.S.*, 1953, **75**, 4834.
Hasek, W.R. *et al, J.A.C.S.*, 1960, **82**, 543.
Stevens, T.E., *J.O.C.*, 1961, **26**, 1627.
White, H.F., *Anal. Chem.*, 1965, **27**, 405 (*pmr, F-19 nmr*)
Kerr, J.A. *et al, J.C.S.(A)*, 1966, 1621.

1,2-Difluoro-1,1,2,2-tetraphenylethane D-1-00251

1,1',1'',1'''-(1,2-Difluoro-1,2-ethanediylidene) tetrakisbenzene, 9CI

[137742-81-5]

$Ph_2CFCFPh_2$

$C_{26}H_{20}F_2$ M 370.4
Cryst. (petrol). Mp 240-241°.

Zupan, M. *et al, J.C.S. Perkin 1*, 1993, 2851 (*synth, pmr, F-19 nmr*)

1,2-Difluoro-1,1,2-triphenylethane D-1-00252

1,1',1''-(1,2-Difluoro-1-ethanyl-2-ylidene) trisbenzene, 9CI

[125440-38-2]

$Ph_2CFCHFPh$

$C_{20}H_{16}F_2$ M 294.3

(±)-*form*
Cryst. (petrol). Mp 120°.

Zupan, M. *et al, J.C.S. Perkin 1*, 1993, 2851 (*synth, pmr, F-19 nmr*)

Diheptyl disulfide, 9CI D-1-00253

[10496-16-9]

$H_3C(CH_2)_6SS(CH_2)_6CH_3$

$C_{14}H_{30}S_2$ M 262.5
Oil. Bp_{12} 165-167°. n_D^{20} 1.4870.

S,S,S',S'-Tetraoxide: Diheptyl disulfone, 9CI
$C_{14}H_{30}O_4S_2$ M 326.5 Plates (hexane). Mp 91.5-92.5°.

Westlake, H.E. *et al, J.A.C.S.*, 1942, **64**, 149 (*synth*)
Allen, P. *et al, J.O.C.*, 1951, **16**, 767 (*disulfone*)
Chorbadjiev, S. *et al, Rev. Roum. Chim.*, 1981, **26**, 1447 (*synth*)
Zhang, Y. *et al, Synth. Commun.*, 1994, **24**, 2893 (*synth, pmr*)

Diheptyl ether D-1-00254

1,1'-Oxybisheptane. Heptyl ether

[629-64-1]

$H_3C(CH_2)_6O(CH_2)_6CH_3$

$C_{14}H_{30}O$ M 214.3
Liq. d 0.80. Bp 256-258°. n_D^{20} 1.4275.

Vogel, A.I., *J.C.S.*, 1948, 618.

Dihexyl disulfide, 9CI D-1-00255

[10496-15-8]

$H_3C(CH_2)_5SS(CH_2)_5CH_3$

$C_{12}H_{26}S_2$ M 234.4
Oil. Bp_{15} 162-166°, $Bp_{0.1}$ 98-100°. n_D^{20} 1.4870.

S,S,S',S'-Tetraoxide: [63450-69-1]. *Dihexyl disulfone, 9CI*
$C_{12}H_{26}O_4S_2$ M 298.4 Plates (hexane). Mp 74.1-74.9°.

Allen, P. *et al, J.O.C.*, 1951, **16**, 767 (*disulfone*)
Chorbadjiev, S. *et al, J. Prakt. Chem.*, 1977, **319**, 1036 (*synth*)
Bittell, J.E. *et al, J.O.C.*, 1978, **43**, 1687 (*synth*)
Kuliev, A.B. *et al, Zh. Org. Khim.*, 1978, **14**, 661; *J. Org. Chem. USSR* (*Engl. Transl.*), 1978, **14**, 611 (*synth*)
Zhang, Y. *et al, Synth. Commun.*, 1994, **24**, 2893 (*synth, pmr*)

Dihexyl ether D-1-00256

1,1'-Oxybishexane. Hexyl ether

[112-58-3]

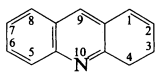
$H_3C(CH_2)_5O(CH_2)_5CH_3$

$C_{12}H_{26}O$ M 186.3
Liq. d 0.79. Bp 219-222°, Bp_5 80-83°. n_D^{20} 1.4204.

Vogel, A.I., *J.C.S.*, 1948, 618.

3,4-Dihydroacridine D-1-00257

[37624-10-5]



$C_{13}H_{11}N$ M 181.2

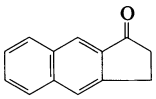
Cryst. (hexane). Mp 45-46°.

Boyd, D.R. *et al*, *J.O.C.*, 1994, **59**, 984 (*synth, pmr*)

2,3-Dihydro-1*H*-benz[*f*]inden-1-one, 9CI D-1-00258

Benz[f]indan-1-one

[109341-49-3]



$C_{13}H_{10}O$ M 182.2

Cryst. (EtOH aq.). Mp 144-145°.

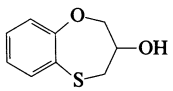
Horner, L. *et al*, *Chem. Ber.*, 1959, **92**, 2953 (*synth*)

Morris, J.L. *et al*, *J.O.C.*, 1994, **59**, 6484 (*synth, pmr*)

3,4-Dihydro-2*H*-1,5-benzooxathiepin-3-ol, 9CI D-1-00259

3,4-Dihydro-3-hydroxy-2H-1,5-benzoxathiepin

[85615-06-1]



$C_9H_{10}O_2S$ M 182.2

(±)-*form*

Cryst. (aq. EtOH). Mp 78°, Mp 93-94°.

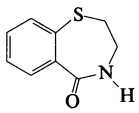
Cabiddu, S. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1983, **14**, 151 (*synth*)

Sugihara, H. *et al*, *Chem. Pharm. Bull.*, 1987, **35**, 1919 (*synth, ir, pmr, ms*)

Ceroni, G. *et al*, *J. Het. Chem.*, 1994, **31**, 1151 (*cryst struct*)

3,4-Dihydro-1,4-benzothiazepin-5(2*H*)-one, 9CI D-1-00260

[14944-00-4]



C_9H_9NOS M 179.2

Cryst. (MeOH or Me_2CO). Mp 191-191.5°.

N-*Me:* [14946-36-2].
$C_{10}H_{11}NOS$ M 193.2 Rods (C_6H_6/petrol). Mp 67-69°.

S-*Oxide:* [23103-66-4].
$C_9H_9NO_2S$ M 195.2 Needles (H_2O); cryst. (MeCN). Mp 233-234° (224°).

S,S-*Dioxide:* [14953-96-9].
$C_9H_9NO_3S$ M 211.2 Leaflets (H_2O). Mp 248-250° (241-241.5°).

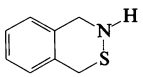
Jokob, F. *et al*, *Chem. Ber.*, 1963, **96**, 88 (*synth*)

Wünsch, K.-H. *et al*, *Chem. Ber.*, 1969, **102**, 1618 (*synth, oxides*)

Nair, M.D. *et al*, *Indian J. Chem.*, 1969, **7**, 862 (*oxides*)

Bose, A.K. *et al*, *J.C.S. Perkin 1*, 1976, 2343 (*synth*)

3,4-Dihydro-1*H*-2,3-benzothiazine D-1-00261



C_8H_9NS M 151.2

S,S-*Dioxide:* [33183-87-8].
$C_8H_9NO_2S$ M 183.2 Cryst. (EtOAc). Mp 142-143°.

N-*Me*, S,S-*dioxide:* [61199-72-2]. *3,4-Dihydro-3-methyl-1H-2,3-benzothiazine 2,2-dioxide, 9CI*
$C_9H_{11}NO_2S$ M 197.2 Cryst. (diisopropyl ether). Mp 74-75°.

N-*Et*, S,S-*dioxide:* [33050-15-6].
$C_{10}H_{13}NO_2S$ M 211.2 Cryst. Mp 70-71°.

N-*Isopropyl*, S,S-*dioxide:* [110654-43-8].
$C_{11}H_{15}NO_2S$ M 225.3 Cryst. (diisopropyl ether). Mp 90-91°.

N-*Benzyl*, S,S-*dioxide:* [110654-44-9].
$C_{15}H_{15}NO_2S$ M 273.3 Cryst. (diisopropyl ether). Mp 84-85°.

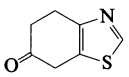
Orazai, O.O. *et al*, *J. Het. Chem.*, 1986, **23**, 1701 (*synth, deriv, pmr, ir*)

Zinczuk, J. *et al*, *Org. Mass Spectrom.*, 1990, **25**, 517 (*ms*)

Rivero, B.E. *et al*, *Acta Cryst. C*, 1991, **47**, 2501 (*cryst struct, dioxide*)

4,7-Dihydro-6(5*H*)-benzothiazolone D-1-00262

[70590-43-1]



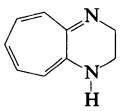
C_7H_7NOS M 153.2

Light yellow waxy solid. $Bp_{0.08}$ 100° (oven).

Kozikowski, A.P. *et al*, *Helv. Chim. Acta*, 1994, **77**, 1256 (*synth, ir, cmr*)

2,3-Dihydro-1*H*-cycloheptapyrazine, 9CI D-1-00263

[120624-12-6]



$C_9H_{10}N_2$ M 146.1

Shows rapid prototropy between two (equivalent) structs. Pale yellow needles. Mp 134°. In general, acylation gives mostly ring-opened products.

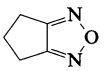
N-*Benzoyl:* [161013-06-5].
$C_{16}H_{14}N_2O$ M 250.2 Deep yellow oil.

N-*Me:* [124293-38-5].
$C_{10}H_{12}N_2$ M 160.2 Red-brown oil.

Nozoe, T. *et al*, *Heterocycles*, 1989, **28**, 733 (*synth, uv, pmr, tautom*)

Kawamata, Y. *et al*, *J. Het. Chem.*, 1994, **31**, 1553.

5,6-Dihydro-4*H*-cyclopenta[*c*]furazan D-1-00264



$C_5H_6N_2O$ M 110.1

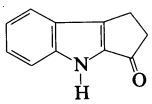
Cryst. (Et_2O). Mp 40.5-41°.

Tokura, N. *et al*, *Bull. Chem. Soc. Jpn.*, 1965, **35**, 722 (*synth*)

Sheremet'ev, A.B., *J. Het. Chem.*, 1995, **32**, 571 (*rev*)

1,4-Dihydrocyclopent[*b*]indol-3(2*H*)-one, 9CI D-1-00265

[16244-15-8]



$C_{11}H_9NO$ M 171.1

Yellow needles (EtOH); prisms (AcOH). Mp 252-252.5°.

Oxime: [22942-83-2].
$C_{11}H_{10}N_2O$ M 186.2 Cryst. (EtOH aq. or MeOH aq.). Mp 162-163°.

Semicarbazone: [22942-85-4].
Mp 226° dec.

N-*Ac:* [65602-71-3].
$C_{13}H_{11}NO_2$ M 213.2 Yellow needles. Mp 151-152°.

N-*Me:* [16244-16-9]. *1,4-Dihydro-4-methylcyclopent*[b]*indol-3*(2H)-*one*
$C_{12}H_{11}NO$ M 185.2 Needles (EtOH). Mp 133-134°.

Elks, J. *et al*, *J.C.S.*, 1944, 624 (*synth*)

Jennings, K.F., *J.C.S.*, 1957, 497 (*synth, uv, ir*)

Uhle, F.C. *et al*, *J.A.C.S.*, 1960, **82**, 1200 (*synth*)

Ishizumi, K. *et al*, *Chem. Pharm. Bull.*, 1967, **15**, 863, 1010 (*synth, N-Me, uv, ir, pmr*)

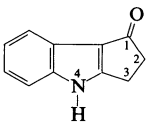
Nagarajan, K. *et al*, *Indian J. Chem.*, 1969, **7**, 319 (*synth, oxime*)

Nagasaka, T. *et al*, *Chem. Pharm. Bull.*, 1977, **25**, 3023 (*N-Ac*)

Teranishi, K. *et al*, *Synthesis*, 1995, 506 (*N-Ac*)

3,4-Dihydrocyclopent[*b*]indol-1(2*H*)-one, 9CI D-1-00266

[61364-20-3]



$C_{11}H_9NO$ M 171.1

Pale tan prisms. Mp 252-253°.

N-*Me:* [50776-26-6]. *3,4-Dihydro-4-methylcyclopent*[b]*indol-1*(2H)-*one, 9CI*
$C_{12}H_{11}NO$ M 185.2 Mp 209-210°.

N-*Me, oxime:* [122852-74-8].
$C_{12}H_{12}N_2O$ M 200.2 Mp 219-224° dec.

Oikawa, Y. *et al*, *J.O.C.*, 1977, **42**, 1213 (*synth, uv*)

Iida, H. *et al*, *J.O.C.*, 1980, **45**, 2938 (*synth*)

Kaneiko, C. *et al*, *Chem. Pharm. Bull.*, 1982, **30**, 74 (*synth, pmr*)

Robinson, B., *J. Het. Chem.*, 1987, **24**, 1321 (*synth, uv*)

3,4-Dihydrocyclopent[*b*]indol-2(1*H*)-one, 9CI D-1-00267

[150670-63-6]

$C_{11}H_9NO$ M 171.1

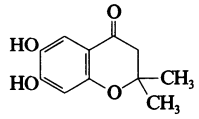
Mp 184-186°.

Franceschetti, L. *et al*, *Tet. Lett.*, 1993, **34**, 3185 (*synth, pmr*)

2,3-Dihydro-6,7-dihydroxy-2,2-dimethyl-4*H*-1-benzopyran-4-one D-1-00268

6,7-Dihydroxy-2,2-dimethylchromanone

[76348-95-3]



$C_{11}H_{12}O_4$ M 208.2
Cryst. (EtOH aq.). Mp 208-209°.

6-Me ether: [74094-45-4]. *2,3-Dihydro-7-hydroxy-6-methoxy-2,2-dimethyl-4H-1-benzopyran-4-one, 9CI*
$C_{12}H_{14}O_4$ M 222.2 Cryst. (MeOH). Mp 113-114° (107°).

7-Me ether: [74094-44-3]. *2,3-Dihydro-6-hydroxy-7-methoxy-2,2-dimethyl-4H-1-benzopyran-4-one, 9CI. 6-Hydroxy-7-methoxy-2,2-dimethylchromanone*
$C_{12}H_{14}O_4$ M 222.2 Mp 98-100°, Mp 136-137°, Mp 150-151° (143-144°).

Di-Me ether: [65383-61-1]. *2,3-Dihydro-6,7-dimethoxy-2,2-dimethyl-4H-1-benzopyran-4-one, 9CI. 6,7-Dimethoxy-2,2-dimethylchromanone*
$C_{13}H_{16}O_4$ M 236.2 Isol. from the leaf resin of *Nama hispidum*. Cryst. Mp 106° (103-104°).

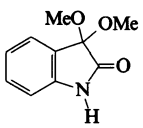
[74094-45-4]

Camps, F. *et al*, *Synthesis*, 1980, 725 (*synth, ethers, pmr, ir*)
Shoja, M., *Acta Cryst. C*, 1988, **44**, 1853 (*cryst struct, deriv*)
Timar, T. *et al*, *J. Het. Chem.*, 1988, **25**, 871 (*synth, pmr, bibl*)
Duddeck, H. *et al*, *Magn. Reson. Chem.*, 1989, **27**, 170 (*O-17 nmr*)
Brown, P.E. *et al*, *J.C.S. Perkin 1*, 1990, 2979 (*di-Me ether*)
Miranda, M.A. *et al*, *Heterocycles*, 1991, **32**, 1159 (*ethers*)
Mulchandani, N.B. *et al*, *Indian J. Chem., Sect. B*, 1992, **31**, 338 (*ether*)
Roitman, J.N. *et al*, *Phytochemistry*, 1993, **33**, 936 (*isol, deriv*)
Timár, T. *et al*, *Synthesis*, 1994, 837 (*6-Me ether*)

1,3-Dihydro-3,3-dimethoxy-2*H*-indol-2-one, 9CI D-1-00269

3,3-Dimethoxy-2-indolinone

[66346-69-8]



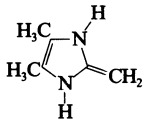
$C_{10}H_{11}NO_3$ M 193.2
Cryst. (CH_2Cl_2/hexane). Mp 94°.

N-Et:
$C_{12}H_{15}NO_3$ M 221.2 $Bp_{0.6}$ 125-128°.

Wenkert, E. *et al*, *Synth. Commun.*, 1977, **7**, 541 (*synth, ir, pmr, ms*)
De, A. *et al*, *Acta Cryst. C*, 1991, **47**, 2384 (*cryst struct*)

2,3-Dihydro-4,5-dimethyl-2-methylene-1*H*-imidazole, 9CI D-1-00270

4,5-Dimethyl-2-methyleneimidazoline



$C_6H_{10}N_2$ M 110.1

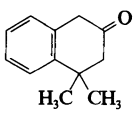
1,3-Di-Me: [151843-01-5].
$C_8H_{14}N_2$ M 138.2 Solid. Highly air-sensitive.

Kuhn, N. *et al*, *Chem. Comm.*, 1993, 1136 (*synth, pmr, cmr, ms, cryst struct*)

3,4-Dihydro-4,4-dimethyl-2(1*H*)-napthalenone D-1-00271

4,4-Dimethyl-2-tetralone

[83810-57-5]



$C_{12}H_{14}O$ M 174.2
Viscous liq. d_4^{23} 1.05. Bp_{16} 149-150°, $Bp_{0.2}$ 91-92°. n_D^{23} 1.5412.

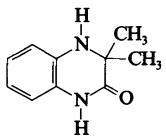
Semicarbazone: Yellow cryst. Mp 181°.

Colonge, J. *et al*, *Bull. Soc. Chim. Fr.*, 1947, 1002 (*synth*)
Vebrel, J. *et al*, *Bull. Soc. Chim. Fr.*, 1982, **II**, 161 (*synth, ir, pmr*)
Pendergast, W. *et al*, *J. Med. Chem.*, 1993, **36**, 2279 (*synth*)

3,4-Dihydro-3,3-dimethyl-2(1*H*)-quinoxalinone, 9CI D-1-00272

1,2,3,4-Tetrahydro-3,3-dimethyl-2-quinoxalinone

[80636-30-2]

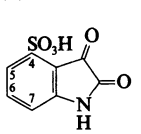


$C_{10}H_{12}N_2O$ M 176.2
Cryst. (CH_2Cl_2/hexane). Mp 179-181° (173-174°).

Hinsberg, O., *Annalen*, 1896, **292**, 245.
Lai, J.T., *Synthesis*, 1982, 71 (*synth, ir, pmr*)
TenBrink, R. *et al*, *J. Med. Chem.*, 1994, **37**, 758 (*synth, pmr*)

2,3-Dihydro-2,3-dioxo-1*H*-indole-4-sulfonic acid D-1-00273

4-Isatinsulfonic acid



$C_8H_5NO_5S$ M 227.1
Microscopic orange-brown cryst. Dec. 183° without melting.

Giovannii, E. *et al*, *Helv. Chim. Acta*, 1957, **31**, 249 (*synth*)

2,3-Dihydro-2,3-dioxo-1*H*-indole-5-sulfonic acid, 9CI D-1-00274

5-Isatinsulfonic acid. 2,3-Dioxo-5-indolinesulfonic acid, 8CI

[7313-70-4]

$C_8H_5NO_5S$ M 227.1
Yellow-brown microcryst. Mp 145-147°.

Chloride: [132898-96-5].
$C_8H_4ClNO_4S$ M 245.6 Yellow powder (Me_2CO/C_6H_6). Mp 150-151°.

Amide: [3456-82-4].
$C_8H_6N_2O_4S$ M 226.2 Cryst. (DMSO aq.). Mp >320°.

[30755-41-0]

Giovannini, E. *et al*, *Helv. Chim. Acta*, 1957, **31**, 249 (*synth*)

2,3-Dihydro-2,3-dioxo-1*H*-indole-6-sulfonic acid D-1-00275

6-Isatinsulfonic acid

$C_8H_5NO_5S$ M 227.1
Orange cryst. Mp >290° dec.

Giovannini, E. *et al*, *Helv. Chim. Acta*, 1957, **31**, 249 (*synth*)

2,3-Dihydro-2,3-dioxo-1*H*-indole-7-sulfonic acid D-1-00276

7-Isatinsulfonic acid

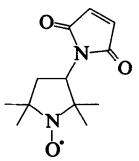
$C_8H_5NO_5S$ M 227.1
Yellow cryst. Mp >350° dec.

Giovannini, E. *et al*, *Helv. Chim. Acta*, 1957, **31**, 249 (*synth*)

3-(2,5-Dihydro-2,5-dioxo-1*H*-pyrrol-2-yl)-2,2,5,5-tetramethyl-1-pyrrolidinyloxy, 9CI D-1-00277

3-Maleimido-2,2,5,5-tetramethyl-1-pyrrolidinyloxy. 3-Maleimido-PROXYL

[5389-27-5]



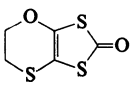
$C_{12}H_{17}N_2O_3$ M 237.2
Free radical. Spin label for thiol groups. Mp 111-113°.

Griffith, O.H. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1966, **55**, 8 (*synth*)
Houstek, J. *et al*, *FEBS Lett.*, 1983, **154**, 185 (*use*)

5,6-Dihydro-1,3-dithiolo[4,5-*b*][1,4]oxathiin-2-one, 9CI D-1-00278

(Dihydro-1,4-oxathiino)-1,3-dithiole-2-one

[156119-23-2]



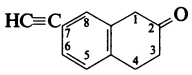
$C_5H_4O_2S_3$ M 192.2

Hellberg, J. *et al*, *Chem. Comm.*, 1994, 817 (*synth, pmr, cmr, ms*)

3,4-Dihydro-7-ethynyl-2(1*H*)-naphthalenone, 9CI D-1-00279

7-Ethynyl-2-tetralone

[139988-09-3]



$C_{12}H_{10}O$ M 170.2

Pendergast, W. *et al*, *J. Med. Chem.*, 1993, **36**, 2279 (*synth, pmr*)

2,3-Dihydro-7-hydroxy-4*H*-1-benzopyran-4-one, 9CI D-1-00280

7-Hydroxy-4-chromanone

[76240-27-2]

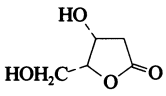
$C_9H_8O_3$ M 164.1
Needles (H_2O). Mp 143°.

Trifluoromethanesulfonyl:
$C_{10}H_7F_3O_5S$ M 296.2 Cryst. Mp 43-44°.

Dann, V.O. *et al*, *Annalen*, 1954, **587**, 16 (*synth*)
Koch, K. *et al*, *J.O.C.*, 1994, **59**, 1216 (*synth, ir, pmr*)

4,5-Dihydro-4-hydroxy-5-(hydroxymethyl)-2(3*H*)-furanone D-1-00281

3-Hydroxy-4-hydroxymethyl-4-butanolide.
3,4,5-Trihydroxypentanoic acid 1,4-lactone



(4*R*,5*R*)-*form*

$C_5H_8O_4$ M 132.1
Satiety-modulating substance in rats.

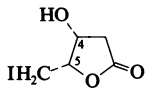
(***4R,5R*)-*form***
Oil. $[\alpha]_D^{24}$ +67.3 (c, 1.01 in MeOH) (+49.3).

(***4S,5R*)-*form***
$[\alpha]_D^{24}$ −4.5 (c, 1.44 in EtOH) (−1.5).

Fernández, M.V. *et al*, *Tetrahedron*, 1990, **46**, 7911 (*synth, pmr, cmr*)
Matsumoto, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1995, **68**, 670 (*synth*)

Dihydro-4-hydroxy-5-(iodomethyl)-2(3*H*)-furanone D-1-00282

3-Hydroxy-4-(iodomethyl)-γ-butyrolactone.
2,5-Dideoxy-5-iodopentonic acid γ-lactone, 9CI



$C_5H_7IO_3$ M 242.0

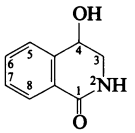
(***4R,5S*)-*form*** [152442-10-9]
D-threo-*form*
Cryst. (hexane/CH_2Cl_2). Mp 68-70°. $[\alpha]_D^{25}$ −39.61 (c, 1.15 in $CHCl_3$).

[81357-33-7, 82166-98-1, 83602-73-7, 86390-93-4, 152442-11-0, 159811-83-3]

Chamberlin, A.R. *et al*, *J.A.C.S.*, 1983, **105**, 5819 (*synth, pmr, ir*)
Takahara, H. *et al*, *J.O.C.*, 1994, **59**, 7201 (*synth, ir, pmr, cmr*)

3,4-Dihydro-4-hydroxy-1(2*H*)-isoquinolinone, 9CI D-1-00283

[23206-20-4]



$C_9H_9NO_2$ M 163.1

(±)-*form*
Cryst. (EtOH aq.). Mp 150-151°, Mp 164-165° (dimorph.).

N-*Me:* [127787-23-9].
$C_{10}H_{11}NO_2$ M 177.2 Cryst. (Me_2CO). Mp 124-126°.

Wilson, J.W. *et al*, *J.O.C.*, 1951, **16**, 800 (*synth*)
Ram, S. *et al*, *Indian J. Chem., Sect. B*, 1978, **16**, 1019 (*synth, ir, pmr*)
Sugimoto, A. *et al*, *Synthesis*, 1995, 431 (*synth, N-Me, ir, pmr, ms*)

3,4-Dihydro-5-hydroxy-1(2*H*)-isoquinolinone, 9CI D-1-00284

[56469-02-4]

$C_9H_9NO_2$ M 163.1
Cryst. (H_2O). Mp 195-198°.

Me ether: [129075-49-6]. *3,4-Dihydro-5-methoxy-1*(2H)*-isoquinolinone*
$C_{10}H_{11}NO_2$ M 177.2 Cryst. (Me_2CO). Mp 146-149°.

Eur. Pat., 355 750, (1990); *CA*, **113**, 132025y (*synth*)
Suto, M.J. *et al*, *Anti-Cancer Drug Des.*, 1991, **6**, 107; *CA*, **115**, 92038n (*Me ether*)

3,4-Dihydro-6-hydroxy-1(2*H*)-isoquinolinone, 9CI D-1-00285

3,4-Dihydro-6-hydroxyisocarbostyril, 8CI

[22245-98-3]

$C_9H_9NO_2$ M 163.1
Cryst. (EtOH). Mp 223-224°.

O-*Ac:* [22245-99-4].
$C_{11}H_{11}NO_3$ M 205.2 Mp 142-143°.

Me ether: [22246-12-4]. *3,4-Dihydro-6-methoxy-1*(2H)*-isoquinolinone*
$C_{10}H_{11}NO_2$ M 177.2 Cryst. (Et_2O or EtOAc). Mp 139-140°.

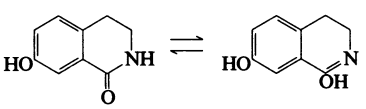
Me ether, N-*Me: 3,4-Dihydro-6-methoxy-2-methyl-1*(2H)*-isoquinolinone*
$C_{11}H_{13}NO_2$ M 191.2 Rhombs (C_6H_6/petrol). Mp 50°.

Gulland, J.M. *et al*, *J.C.S.*, 1929, 1791 (*Me ether, N-Me*)
Tomita, M. *et al*, *J.C.S.*(*C*), 1969, 183 (*synth, Ac, Me ether*)
Weimar, C. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1991, **324**, 509 (*Me ether*)

3,4-Dihydro-7-hydroxy-1(2*H*)-isoquinolinone, 9CI D-1-00286

3,4-Dihydro-7-hydroxyisocarbostyril, 8CI

[22246-05-5]



$C_9H_9NO_2$ M 163.1
Cryst. (Me_2CO). Mp 200-202° dec.

O-*Ac:* [22245-93-8].
$C_{11}H_{11}NO_3$ M 205.2 Mp 140-141°.

Me ether: [22246-04-4]. *3,4-Dihydro-7-methoxy-1*(2H)*-isoquinolinone*
$C_{10}H_{11}NO_2$ M 177.2 Cryst. (Et_2O or EtOAc/hexane). Mp 86°, Mp 112-113°.

Tomita, M. *et al*, *J.C.S.*(*C*), 1969, 183 (*synth, Ac, Me ether*)
Ajao, J.F. *et al*, *J. Het. Chem.*, 1985, **22**, 327 (*Me ether*)
Weimar, C. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1991, **324**, 509 (*Me ether*)

3,4-Dihydro-8-hydroxy-1(2*H*)-isoquinolinone, 9CI D-1-00287

[135329-20-3]

$C_9H_9NO_2$ M 163.1
Mp 147-149° (hemihydrate).

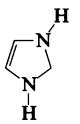
Me ether: [74904-29-3]. *3,4-Dihydro-8-methoxy-1*(2H)*-isoquinolinone*
$C_{10}H_{11}NO_2$ M 177.2 Cryst. (C_6H_6). Mp 148-149°.

Kashdan, D.S. *et al*, *J.O.C.*, 1982, **47**, 2638 (*Me ether*)
Suto, M.J. *et al*, *Anti-Cancer Drug Des.*, 1991, **6**, 107; *CA*, **115**, 92038n (*synth, pmr*)
Shanker, P.S. *et al*, *Indian J. Chem., Sect. B*, 1993, **32**, 1209 (*Me ether*)

2,3-Dihydro-1*H*-imidazole, 9CI D-1-00288

4-Imidazoline

[6569-26-2]

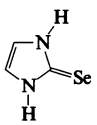


$C_3H_6N_2$ M 70.0

1,3-Di-Ac: [10284-52-3].
$C_7H_{10}N_2O_2$ M 154.1 Cryst. (MeOH). Mp 249-251°.

Plath, M.W. *et al*, *Synthesis*, 1990, 951 (*synth, ir, uv, pmr, cmr, cryst struct, deriv*)

1,3-Dihydro-2*H*-imidazole-2-selone D-1-00289



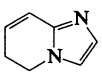
$C_3H_4N_2Se$ M 147.0

N-*Me:* [157997-38-1]. *1,3-Dihydro-1-methyl-2H-imidazole-2-selone, 9CI*
$C_4H_6N_2Se$ M 161.0 Orange cryst. solid (EtOAc/hexanes). Mp 142°.

Guziec, L.J. *et al*, *J.O.C.*, 1994, **59**, 4691 (*1-Me, synth, ir, pmr, cmr*)

5,6-Dihydroimidazo[1,2-*a*]pyridine, 9CI D-1-00290

[156817-69-5]

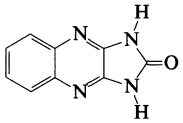


$C_7H_8N_2$ M 120.1

Hua, D.H. *et al*, *J.O.C.*, 1994, **59**, 5084 (*synth, pmr, cmr*)

1,3-Dihydro-2*H*-imidazo[4,5-*b*]quinoxalin-2-one D-1-00291

[54108-04-2]



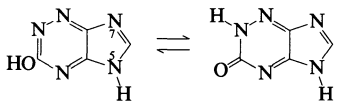
$C_9H_6N_4O$ M 186.1
Cryst. Mp >330°.

Schipper, E. *et al*, *J.A.C.S.*, 1951, **73**, 5672.
Obafemi, C.A. *et al*, *Helv. Chim. Acta*, 1994, **77**, 1549 (*synth, uv, pmr*)

1,2-Dihydro-3*H*-imidazo[4,5-*e*]-1,2,4-triazin-3-one, 9CI D-1-00292

Imidazo[4,5-e]-1,2,4-triazin-3(2H)-one. 3-Hydroxyimidazo[4,5-e]-1,2,4-triazine. Imidazo[4,5-e][1,2,4]triazin-3-ol. 6-Aza-2-purinol

[160663-25-2]



$C_4H_3N_5O$ M 137.1
NH-form predominates. Cryst. (EtOH or MeOH). Mp 246° slow dec. Undergoes covalent addn. of H_2O or alcohols.

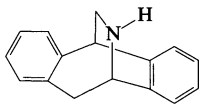
5-Me: [160663-26-3]. *2,5-Dihydro-5-methyl-3H-imidazo-[4,5-e]-1,2,4-triazin-3-one, 9CI*
$C_5H_5N_5O$ M 151.1 Cryst. (EtOH/MeOH). Mp 270° slow dec. Undergoes covalent addn. of H_2O or alcohols.

7-Me: [130446-48-9]. *2,7-Dihydro-7-methyl-3H-imidazo[4,5-e]-1,2,4-triazin-3-one, 9CI*
$C_5H_5N_5O$ M 151.1 Solid. Mp 218° slow dec. Could not be recryst. Undergoes strong covalent addn. of H_2O or alcohols.

Tzeng, C. *et al*, *J.C.S. Perkin 2*, 1994, 2563 (*synth, uv*)

10,11-Dihydro-10,5-(iminomethano)-5*H*-dibenzo[*a,d*]cycloheptene, 9CI D-1-00293

[27569-65-9]



(+)-*form*

$C_{16}H_{15}N$ M 221.3
(+)-***form*** [135029-85-5]
Cryst. Mp 79-85°. $[\alpha]_D^{25}$ +165 (c, 1 in EtOH).

N-*Me:* [135579-62-3].
$C_{17}H_{17}N$ M 235.3 Oil. $[\alpha]_D^{25}$ +189 (c, 1 in EtOH).

(±)-***form*** [131475-40-6]
Cryst. (C_6H_6/Me_2CO). Mp 79°.

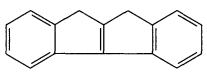
N-*Ac:* [131475-56-4].
$C_{18}H_{17}NO$ M 263.3 Cryst. (MeOH). Mp 205°.

[17749-16-5, 23099-06-1, 27569-80-8, 67576-52-7, 68962-92-5]

Dobson, T.A. *et al*, *Tet. Lett.*, 1967, 4139 (*synth*)
Suzuki, T. *et al*, *Chem. Pharm. Bull.*, 1986, **34**, 1888 (*synth, pmr*)
Yasuda, M. *et al*, *Heterocycles*, 1992, **34**, 965 (*synth, pmr, cmr*)
Gee, K.R. *et al*, *J. Med. Chem.*, 1993, **36**, 1938.

9,10-Dihydroindeno[1,2-*a*]indene D-1-00294

[7263-76-5]

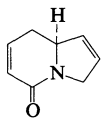


$C_{16}H_{12}$ M 204.2
Cryst. (EtOH). Mp 135°.

Japan. Pat., 68 00 509, (1968); *CA*, **70**, 11411f (*synth*)
Uyehara, T. *et al*, *Chem. Lett.*, 1977, 1233 (*pmr, anion*)

8,8*a*-Dihydro-5(3*H*)-indolizinone, 9CI D-1-00295

3,5,8,8a-Tetrahydro-5-oxoindolizine



C_8H_9NO M 135.1
Intermed. for prepn. of indolizidine alkaloids.

(*S*)-***form*** [151983-41-4]
Oil. $[\alpha]_D^{24}$ −331 (c, 1.18 in CH_2Cl_2) (86% ee).

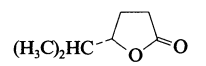
[151983-36-7]

Nukui, S. *et al*, *Tet. Lett.*, 1993, **34**, 4965 (*synth*)
Sato, Y. *et al*, *Tetrahedron*, 1994, **50**, 371 (*synth*)
Nukui, S. *et al*, *J.O.C.*, 1995, **60**, 398 (*use*)

Dihydro-5-isopropyl-2(3*H*)-furanone D-1-00296

Dihydro-5-(1-methylethyl)-2(3H)-furanone, 9CI. γ-Isopropyl-γ-butyrolactone

[38624-29-2]



(*S*)-*form*

$C_7H_{12}O_2$ M 128.1
(*S*)-***form*** [154799-15-2]
Bp_{52} 124-126°. $[\alpha]_D^{25}$ +43.5 (c, 1.92 in $CHCl_3$).

(±)-***form***
$Bp_{0.5}$ 56°. n_D^{20} 1.4416.

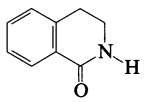
[144731-12-4]

Lunstead, R.P. *et al*, *J.C.S.*, 1933, 580 (*synth*)
Loewen, P.C. *et al*, *Can. J. Chem.*, 1972, **50**, 1502 (*synth*)
Brown, H.C. *et al*, *J.O.C.*, 1994, **59**, 365 (*S-form*)

3,4-Dihydro-1(2*H*)-isoquinolinone, 9CI D-1-00297

3,4-Dihydroisocarbostyril

[1196-38-9]



C_9H_9NO M 147.1
Cryst. (MeOH aq.). Mp 58°. $Bp_{0.1}$ 125-127°.

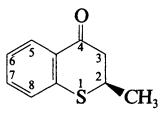
N-*Me:*
$C_{10}H_{11}NO$ M 161.2 Liq. Bp_6 157°, $Bp_{0.4}$ 118°.

Schneider, W. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1958, **291**, 560 (*synth, N-Me*)
Davies, R.V. *et al*, *J.C.S. Perkin 1*, 1978, 180 (*synth, ir*)
Norman, M.H. *et al*, *J. Med. Chem.*, 1994, **37**, 2552 (*synth, pmr*)

2,3-Dihydro-2-methyl-4*H*-1-benzothiopyran-4-one, 9CI D-1-00298

2-Methylthiochroman-4-one, 8CI

[826-86-8]



(*R*)-*form*

$C_{10}H_{10}OS$ M 178.2
(*R*)-***form*** [135587-65-4]
Liq. $[\alpha]_D$ +159.10 (c, 1.67 in $CHCl_3$) (85% ee).

Oxime: [135587-66-5].
$C_{10}H_{11}NOS$ M 193.2 Cryst. (EtOH). $[\alpha]_D$ +61.82 (c, 1.22 in $CHCl_3$).

(±)-***form***
Oil. Mp 18-19°. Bp_9 146-147°.

Semicarbazone: Needles (EtOH). Mp 167-168°.

S-*Oxide:* [23086-34-2].
$C_{10}H_{10}O_2S$ M 194.2 Cryst. (C_6H_6). Mp 109-110°.

S,S-*Dioxide:* [16808-50-7].
$C_{10}H_{10}O_3S$ M 210.2 Cryst. (EtOH). Mp 127-128°.

Krollpfeiffer, F. *et al*, *Ber.*, 1925, **58**, 1654 (*synth*)
Petropoulos, J.C. *et al*, *J.A.C.S.*, 1953, **75**, 1130 (*synth*)
Harrison, A.G. *et al*, *Org. Mass Spectrom.*, 1970, **3**, 899 (*ms*)
Chauhan, M.S. *et al*, *Can. J. Chem.*, 1975, **53**, 2880 (*cmr*)
Kumar, A. *et al*, *Indian J. Chem., Sect. B*, 1992, **31**, 803 (*synth, ir, pmr*)
Clayton, S.E. *et al*, *Tetrahedron*, 1993, **49**, 939 (*synth, pmr*)
Kumar, P. *et al*, *Synth. Commun.*, 1994, **24**, 3297 (*synth, ir, pmr, ms*)

2,3-Dihydro-3-methyl-4*H*-1-benzothiopyran-4-one, 9CI D-1-00299

3-Methylthiochroman-4-one, 8CI

[771-17-5]

$C_{10}H_{10}OS$ M 178.2
(±)-***form*** [127847-86-3]
Needles (pentane). Mp 41-42°. Bp_{10} 146-150°.

Oxime: [14110-50-0].
$C_{10}H_{11}NOS$ M 193.2 Mp 133-134°.

S-*Oxide:* [29373-04-4].
$C_{10}H_{10}O_2S$ M 194.2 Needles (petrol); cryst. (C_6H_6/hexane). Mp 116-117°.

S,S-*Dioxide:* [16723-50-5].
$C_{10}H_{10}O_3S$ M 210.2 Cryst. (EtOH). Mp 146-147°.

Petropoulos, J.C. *et al, J.A.C.S.*, 1953, **75**, 1130 (*synth*)
Harrison, A.G. *et al, Org. Mass Spectrom.*, 1970, **3**, 899 (*ms*)
Chauhan, M.S. *et al, Can. J. Chem.*, 1975, **53**, 2880 (*oxide, cmr*)
Thomson, R.H. *et al, J.C.S. Perkin 1*, 1982, 395 (*oxide, synth*)

2,3-Dihydro-5-methyl-4*H*-1-benzothiopyran-4-one, 9CI D-1-00300

5-Methylthiochroman-4-one, 8CI

[13735-17-6]

$C_{10}H_{10}OS$ M 178.2
Cryst. (petrol). Mp 34-35°. $Bp_{2.5}$ 124°.

S-*Oxide:*
$C_{10}H_{10}O_2S$ M 194.2 Cryst. (C_6H_6/petrol). Mp 112-113°.

S,S-*Dioxide:* [16723-52-7].
$C_{10}H_{10}O_3S$ M 210.2 Cryst. (MeOH). Mp 130-132°.

Degani, I. *et al, Boll. Sci. Fac. Chim. Ind. Bologna*, 1966, **24**, 75; *CA*, **66**, 46292n (*synth*)
Thakkar, S.M. *et al, Curr. Sci.*, 1976, **45**, 178 (*synth, pmr*)

2,3-Dihydro-6-methyl-4*H*-1-benzothiopyran-4-one, 9CI D-1-00301

6-Methylthiochroman-4-one, 8CI

[6948-34-1]

$C_{10}H_{10}OS$ M 178.2
Leaflets or plates (petrol). Mp 41-42°.
Semicarbazone: Leaflets (EtOH). Mp 235°.
S-*Oxide:* [42244-87-1].
$C_{10}H_{10}O_2S$ M 194.2 Cryst. (C_6H_6/petrol). Mp 111-113° (110-111°).

Arndt, F. *et al, Ber.*, 1923, **56**, 1269 (*synth*)
Krollpfeiffer, F. *et al, Ber.*, 1923, **56**, 1818 (*synth*)
Degani, I. *et al, Boll. Sci. Fac. Chim. Ind. Bologna*, 1966, **24**, 75; *CA*, **66**, 46292n (*synth*)
Chauhan, M.S. *et al, Can. J. Chem.*, 1975, **53**, 2880 (*cmr*)
Still, I.W.J. *et al, Can. J. Chem.*, 1976, **54**, 455 (*oxide, synth*)

2,3-Dihydro-7-methyl-4*H*-1-benzothiopyran-4-one D-1-00302

7-Methylthiochroman-4-one, 8CI

[13735-18-7]

$C_{10}H_{10}OS$ M 178.2
Cryst. (petrol). Mp 51-52°. $Bp_{2.5}$ 146°.

S,S-*Dioxide:*
$C_{10}H_{10}O_3S$ M 210.2 Cryst. (EtOH). Mp 159-160°.

Degani, I. *et al, Boll. Sci. Fac. Chim. Ind. Bologna*, 1966, **24**, 75; *CA*, **66**, 46292n (*synth*)
Thakkar, S.M. *et al, Curr. Sci.*, 1976, **45**, 178 (*synth, pmr*)

2,3-Dihydro-8-methyl-4*H*-1-benzothiopyran-4-one, 9CI D-1-00303

8-Methylthiochroman-4-one, 8CI

[29373-02-2]

$C_{10}H_{10}OS$ M 178.2
Pale yellow or tan plates (MeOH aq.). Mp 65°. Bp_{14} 171.5°.

Oxime: [94281-47-7].
$C_{10}H_{11}NOS$ M 193.2 Needles (C_6H_6/petrol). Mp 139.5-140°.

Semicarbazone: [54246-52-5].
Prisms (EtOH). Mp 245°.

S-*Oxide:* [29399-51-7].
$C_{10}H_{10}O_2S$ M 194.2 Cryst. (C_6H_6/petrol). Mp 83-84°.

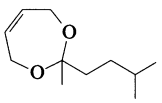
S,S-*Dioxide:*
$C_{10}H_{10}O_3S$ M 210.2 Cryst. (EtOH). Mp 124-125°.

Hurd, C.D. *et al, J.A.C.S.*, 1954, **76**, 5065 (*synth*)
Cagniant, P. *et al, C. R. Hebd. Seances Acad. Sci.*, 1961, **253**, 1702 (*props, derivs*)
Still, I.W.J. *et al, J.O.C.*, 1968, **33**, 2731 (*dioxide*)
Harrison, A.G. *et al, Org. Mass Spectrom.*, 1970, **3**, 899 (*ms*)
Ricci, A. *et al, J. Het. Chem.*, 1974, **11**, 515 (*synth*)
Chauhan, M.S. *et al, Can. J. Chem.*, 1975, **53**, 2880 (*cmr*)

4,7-Dihydro-2-methyl-2-(3-methylbutyl)-1,3-dioxepin, 9CI D-1-00304

4,7-Dihydro-2-isopentyl-2-methyl-1,3-dioxepin. Ambersage

[53338-05-9]



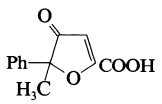
$C_{11}H_{20}O_2$ M 184.2
Used in perfumery to enhance fresh odours. Liq. with fresh lavender-fruity-citrus odour. d 0.94.

U.S. Pat., 3 396 398, (1976); *CA*, **84**, 135736z.

4,5-Dihydro-5-methyl-4-oxo-5-phenyl-2-furancarboxylic acid, 9CI D-1-00305

***Acifran, INN, USAN.** Reductol. AY 25712*

[72420-38-3]



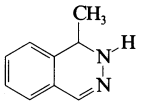
$C_{12}H_{10}O_4$ M 218.2
Antihyperlipidaemic agent.
▶ LD_{50} (rat, orl) 3000 mg/kg. LU0222000.

(+)-***form*** [77103-91-4]
Cryst. (Et_2O). Mp 87-89°. $[\alpha]_D^{25}$ +146.4 (c, 2 in MeOH).

(±)-***form*** [82720-24-9]
Mp 176°.

Cayen, M.N. *et al, Atherosclerosis (Shannon, Irel.)*, 1982, **45**, 267, 281 (*pharmacol*)
Jirkovsky, I. *et al, J. Med. Chem.*, 1982, **25**, 1154 (*synth, pharmacol, resoln*)
Gonzalez, R. *et al, Clin. Biochem.*, 1983, **16**, 244 (*hplc*)
Hunninghake, D.B. *et al, Clin. Pharmacol. Ther. (St. Louis)*, 1985, **38**, 313 (*clin trial*)
Cayen, M.N. *et al, Xenobiotica*, 1986, **16**, 251 (*metab*)
Cayen, M.N. *et al, Clin. Pharmacol. Ther. (St. Louis)*, 1990, **47**, 50 (*pharmacokinet, metab*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 983.

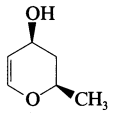
1,2-Dihydro-1-methylphthalazine D-1-00306



$C_9H_{10}N_2$ M 146.1
2-Me: 1,2-Dihydro-1,2-dimethylphthalazine
$C_{10}H_{12}N_2$ M 160.2 Oil.

Ruxer, J.M. *et al, J. Het. Chem.*, 1995, **32**, 643 (*synth, pmr, cmr, ir*)

3,4-Dihydro-2-methyl-2*H*-pyran-4-ol D-1-00307



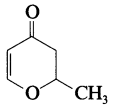
$C_6H_{10}O_2$ M 114.1
(***2RS,4SR*)-*form***
(±)-cis-*form*
Oil.

Ac:
$C_8H_{12}O_3$ M 156.1 Oil. Bp_5 100°.
Me ether: 3,4-Dihydro-4-methoxy-2-methyl-2H-pyran
$C_7H_{12}O_2$ M 128.1 Oil.

Danishefsky, S. *et al, J.O.C.*, 1982, **47**, 1597 (*synth*)
Varelis, P. *et al, Aust. J. Chem.*, 1994, **47**, 1735 (*synth, pmr*)

2,3-Dihydro-2-methyl-4*H*-pyran-4-one, 9CI D-1-00308

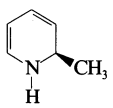
[19185-89-8]



$C_6H_8O_2$ M 112.1
(±)-***form***
Oil. Bp_{23} 180°.

Danishefsky, S. *et al, J.O.C.*, 1982, **47**, 1597 (*synth*)
Varelis, P. *et al, Aust. J. Chem.*, 1994, **47**, 1735 (*synth, pmr*)

1,2-Dihydro-2-methylpyridine D-1-00309



C_6H_9N M 95.1
(***R*)-*form***
N-*Benzyloxycarbonyl: Benzyl 1,2-dihydro-2-methyl-1-pyridinecarboxylate*
$C_{14}H_{15}NO_2$ M 229.2 Yellow oil. $[\alpha]_D$ −546 (c, 0.61 in $CHCl_3$).

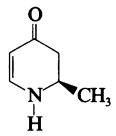
(*S*)-*form*

N-*Benzyloxycarbonyl:*

$C_{14}H_{15}NO_2$ M 229.2 Yellow oil. $[\alpha]_D^{20}$ +588 (c, 0.6 in $CHCl_3$).

Streith, J. *et al*, *Helv. Chim. Acta*, 1995, **78**, 61.

2,3-Dihydro-2-methyl-4(1*H*)-pyridinone, 9CI D-1-00310



(*R*)-*form*

C_6H_9NO M 111.1

(*R*)-*form* [157034-64-5]

Yellow oil. $[\alpha]_D^{20}$ +495 (c, 1.4 in $CHCl_3$).

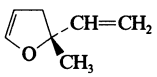
(*S*)-*form* [168105-21-3]

Yellow oil. $[\alpha]_D^{20}$ −487 (c, 1.3 in $CHCl_3$).

Streith, J. *et al*, *Helv. Chim. Acta*, 1995, **78**, 61 (*synth, ir, pmr, cmr*)

2,3-Dihydro-2-methyl-2-vinylfuran D-1-00311

2-Ethenyl-2,3-dihydro-2-methylfuran, 9CI



$C_7H_{10}O$ M 110.1

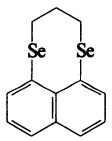
(*R*)-*form* [152999-69-4]

Intermed. for terpene syntheses. Oil. Bp_{10} 70° (bulb). $[\alpha]_D^{20}$ +0.42 (c, 0.74 in $CHCl_3$).

Lord, M.D. *et al*, *J.O.C.*, 1995, **60**, 191 (*synth, ir, pmr, cmr*)

3,4-Dihydro-2*H*-naphtho[1,8-*bc*]-1,5-diselenocin, 9CI D-1-00312

[143952-82-3]



$C_{13}H_{12}Se_2$ M 326.1

Cryst. Mp 92°.

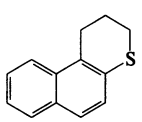
Monoxide: [152193-57-2].

$C_{13}H_{12}OSe_2$ M 342.1 Cryst. Mp 149-151°.

Fujihara, H. *et al*, *J.C.S. Perkin 1*, 1993, 2145 (*synth, pmr, cmr*)

2,3-Dihydro-1*H*-naphtho[2,1-*b*]thiopyran D-1-00313

[5395-24-4]



$C_{13}H_{12}S$ M 200.3

Needles (hexane). Mp 96.5-97°.

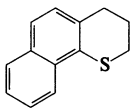
Takido, T. *et al*, *J. Het. Chem.*, 1995, **32**, 687 (*synth, pmr*)

3,4-Dihydro-2*H*-naphtho[1,2-*b*]thiopyran, 9CI D-1-00314

Updated Entry replacing D-0-06383

7,8-Benzothiochroman

[7571-04-2]



$C_{13}H_{12}S$ M 200.3

Liq. Bp_4 159-163°.

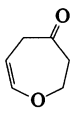
Campaigne, E. *et al*, *J.O.C.*, 1964, **29**, 2373 (*synth*)

Still, I.W.J. *et al*, *Can. J. Chem.*, 1981, **59**, 199 (*pmr*)

Takido, T. *et al*, *J. Het. Chem.*, 1995, **32**, 687 (*synth, pmr*)

2,3-Dihydro-4(5*H*)-oxepinone, 9CI D-1-00315

[111292-47-8]



$C_6H_8O_2$ M 112.1

Pale orange oil.

Kirmse, W. *et al*, *Chem. Ber.*, 1987, **121**, 485 (*synth, pmr, ir*)

Reissig, H.U. *et al*, *Chem. Ber.*, 1994, **127**, 2337 (*synth, pmr, cmr*)

6,7-Dihydro-2(3*H*)-oxepinone, 9CI D-1-00316

3-Hexen-6-olide

[102575-06-4]

$C_6H_8O_2$ M 112.1

Oil.

Le Floc'h, Y. *et al*, *Bull. Soc. Chim. Fr.*, 1991, 742 (*synth, ir, pmr, cmr, ms*)

6,7-Dihydro-2(5*H*)-oxepinone, 9CI D-1-00317

2-Hexen-6-olide

[57205-07-9]

$C_6H_8O_2$ M 112.1

Oil. $Bp_{0.1}$ 68-69°.

Fleming, I. *et al*, *J.C.S. Perkin 1*, 1984, 1815 (*synth, pmr, ir, ms*)

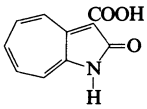
Moriarty, R.M. *et al*, *Tet. Lett.*, 1990, **31**, 197 (*synth, pmr, ir*)

Le Floc'h, Y. *et al*, *Bull. Soc. Chim. Fr.*, 1991, 742 (*synth, ir, pmr, cmr, ms*)

1,2-Dihydro-2-oxocyclohepta[*b*]pyrrole-3-carboxylic acid, 9CI D-1-00318

3-Carboxy-1-aza-2(1H)-azulenone. 3-Carboxycyclohepta[b]pyrrol-2(1H)-one

[20884-33-7]



$C_{10}H_7NO_3$ M 189.1

Cryst. (MeOH). Mp 200°.

Et ester: [1210-27-1].

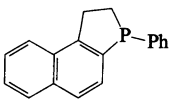
$C_{12}H_{11}NO_3$ M 217.2 Cryst. (EtOH/EtOAc). Mp 183.5-185°.

Nitrile: [1435-20-7]. *1,2-Dihydro-2-oxocyclohepta[b]pyrrole-3-carbonitrile, 9CI. 3-Cyano-1-aza-2(1H)-azulenone*

$C_{10}H_6N_2O$ M 170.1 Solid. Mp >290°.

Nagahara, M. *et al*, *Chem. Pharm. Bull.*, 1994, **42**, 2491.

2,3-Dihydro-3-phenyl-1*H*-benzo[*e*]phosphindole D-1-00319



$C_{18}H_{15}P$ M 262.2

P-*Oxide:* [70610-32-1].

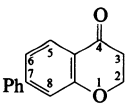
$C_{18}H_{15}OP$ M 278.2 Solid. Mp 200-202°.

Orton, W.L. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1979, **5**, 349 (*synth, cmr, P-31 nmr*)

2,3-Dihydro-7-phenyl-4*H*-1-benzopyran-4-one D-1-00320

7-Phenyl-4-chromanone

[153535-52-5]



$C_{15}H_{12}O_2$ M 224.2

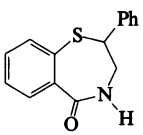
Yellow needles (isopropyl ether). Mp 109°.

Koch, K. *et al*, *J.O.C.*, 1994, **59**, 1216 (*synth, pmr, ir, ms*)

3,4-Dihydro-2-phenyl-1,4-benzothiazepin-5(2*H*)-one, 9CI, 8CI D-1-00321

2,3-Dihydro-2-phenyl-1,4-benzothiazepin-5(4H)-one, 8CI

[17785-40-9]



$C_{15}H_{13}NOS$ M 255.3

(±)-*form*

Cryst. (MeCN). Mp 186-188°.

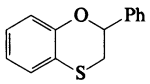
S-*Oxide:* [73859-97-9].

$C_{15}H_{13}NO_2S$ M 271.3 Mp 290° dec.

Krapcho, J. *et al, J. Med. Chem.*, 1968, **11**, 361 (*synth, ir*)
U.K. Pat., 1 181 571, (1970); *CA*, **72**, 100778q (*synth*)
Duddeck, H. *et al, Annalen*, 1985, 869 (*cmr*)
Pócsfalvi, G. *et al, Org. Mass Spectrom.*, 1994, **29**, 303 (*ms*)
Kaye, P.T. *et al, Synth. Commun.*, 1995, **25**, 1495 (*synth, ir, pmr, cmr*)

2,3-Dihydro-2-phenyl-1,4-benzoxathiin D-1-00322

2-Phenyl-1,4-benzoxathiane



$C_{14}H_{12}OS$ M 228.3

(±)-*form*
Oil.

Arnoldi, A. *et al, J.C.S. Perkin 1*, 1994, 1241 (*synth, pmr*)

4,5-Dihydro-2-phenylimidazole D-1-00323

2-Phenyl-Δ^2-imidazoline

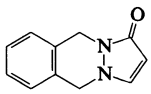
[936-49-2]

$C_9H_{10}N_2$ M 146.1
Cryst. (cyclohexane). Mp 100-101° (97-99°).

Ewin, G. *et al, Aust. J. Chem.*, 1975, **28**, 909 (*synth*)
Egg, H. *et al, J. Het. Chem.*, 1995, **32**, 655 (*synth*)

5,10-Dihydro-1*H*-pyrazolo[1,2-*b*]phthalazin-1-one, 9CI D-1-00324

[169266-86-8]

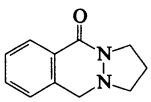


$C_{11}H_{10}N_2O$ M 186.2
Mp 121-124° dec.

Arán, V.J. *et al, Annalen*, 1995, 817 (*synth, pmr, cmr*)

2,3-Dihydro-1*H*-pyrazolo[1,2-*b*]phthalazin-5(10*H*)-one D-1-00325

[28690-02-0]



$C_{11}H_{12}N_2O$ M 188.2
Pale yellow liq. Bp_3 167-170°.

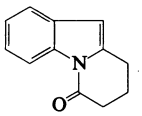
Picrate: [28690-03-1].
Yellow leaflets (EtOH). Mp 209-212° dec.

Nakamura, A. *et al, Chem. Pharm. Bull.*, 1970, **18**, 1526 (*synth*)

8,9-Dihydropyrido[1,2-*a*]indol-6(7*H*)-one, 9CI D-1-00326

6,7,8,9-Tetrahydropyrido[1,2-a]indol-6-one

[91486-93-0]



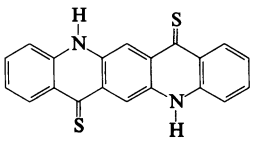
$C_{12}H_{11}NO$ M 185.2
Plates (MeOH). Mp 79-81°.

Crenshaw, M.D. *et al, J. Het. Chem.*, 1984, **21**, 623 (*synth*)
Kato, M. *et al, Chem. Pharm. Bull.*, 1995, **43**, 1346 (*synth, pmr*)

5,12-Dihydroquino[2,3-*b*]acridine-7,14-dithione D-1-00327

5,7,12,14-Tetrahydroquinolino[2,3-b]acridine-7,14-dithione. Dithioquinacridone. Thioquinacridone

[117396-45-9]

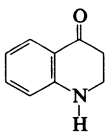


$C_{20}H_{12}N_2S_2$ M 344.4
Patented for use of its near-ir absorption in information storage systems.

Eur. Pat., 267 873, (1988) (*Ciba-Geigy*); *CA*, **109**, 192170u (*synth, use*)
Mizuguchi, J. *et al, Acta Cryst. C*, 1992, **48**, 1553 (*cryst struct*)
Mizuguchi, J. *et al, Ber. Bunsen-Ges. Phys. Chem.*, 1994, **98**, 19 (*uv*)

2,3-Dihydro-4(1*H*)-quinolinone, 9CI D-1-00328

[4295-36-7]



C_9H_9NO M 147.1
Pale yellow leaflets. Mp 43-44.5°. $Bp_{0.2}$ 100°.

N-*Ac:* [64142-63-8].
$C_{11}H_{11}NO_2$ M 189.2 Prisms. Mp 94° (85°). Bp_{17} 206-210°.

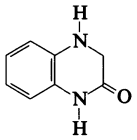
N-*Me:* [1198-15-8].
$C_{10}H_{11}NO$ M 161.2 Yellow oil. Bp_8 185-190°.

Clemo, G.R. *et al, J.C.S.*, 1924, **125**, 1608; 1930, 2133 (*synth, N-Ac*)
Johnson, W.S. *et al, J.A.C.S.*, 1949, **71**, 1901 (*synth*)
Collins, R.F., *J.C.S.*, 1960, 2053 (*synth, N-Ac*)
Maitte, P. *et al, J. Het. Chem.*, 1985, **22**, 713 (*synth, ir, pmr*)
Antus, S. *et al, Annalen*, 1994, 911 (*N-Ac*)

3,4-Dihydro-2(1*H*)-quinoxalinone, 9CI D-1-00329

1,2,3,4-Tetrahydro-2-quinoxalinone

[59564-59-9]



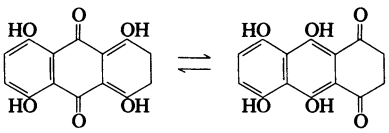
$C_8H_8N_2O$ M 148.1
Cryst. ($EtOAc/CH_2Cl_2$). Mp 136-138°.

TenBrink, R.E. *et al, J. Med. Chem.*, 1994, **37**, 758 (*synth, ir, pmr*)

2,3-Dihydro-1,4,5,8-tetrahydroxyanthraquinone D-1-00330

1,2-Dihydro-1,4,5,8-tetrahydroxy-9,10-anthracenedione, 9CI. Leuco-1,4,5,8-tetrahydroxyanthraquinone. 5,8-Dihydroxyleucoquinizarin

[81-59-4]



$C_{14}H_{10}O_6$ M 274.2
Intermediate for anthraquinone dyes. Bronze leaflets or needles (AcOH). Mp 230-235° dec., Mp >290° dec.

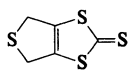
Tetra-Ac:
$C_{22}H_{18}O_{10}$ M 442.3 Yellow needles (AcOH). Mp 266° dec.

[28932-22-1]

Marshall, P.G., *J.C.S.*, 1937, 254 (*synth*)
Allen, C.F.H. *et al, J.O.C.*, 1941, **6**, 732 (*synth*)
Bruce, D.B. *et al, J.C.S.*, 1952, 2759 (*synth, tetra-Ac, ir*)
Chang, P. *et al, Synth. Commun.*, 1995, **25**, 1893 (*synth, ir, ms*)

4,6-Dihydrothieno[3,4-*d*]-1,3-dithiole-2-thione, 9CI D-1-00331

[127501-72-8]



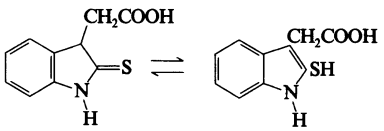
$C_5H_4S_4$ M 192.3
Yellow solid (CCl_4/hexane). Mp 131-134°.

Rovira, C. *et al, J.O.C.*, 1994, **59**, 3307 (*synth, pmr, cmr, ir, uv*)

2,3-Dihydro-2-thioxo-1*H*-indole-3-acetic acid, 9CI D-1-00332

2-Mercapto-1H-indole-3-acetic acid

[149286-91-9]



$C_{10}H_9NO_2S$ M 207.2
Yellow needles. Mp 170-171° (166-168°).

Me ester: [69261-17-2].

$C_{11}H_{11}NO_2S$ M 221.2 Cryst. (MeOH). Mp 150-152°.

Thione-form

N-*Me:* [149286-92-0].
$C_{11}H_{11}NO_2S$ M 221.2 Cryst. (CH_2Cl_2/petrol). Mp 150-153°.

N-*Me, Me ester:* [149286-93-1].
$C_{12}H_{13}NO_2S$ M 235.3 Cryst. (C_6H_6/petrol). Mp 68-70°.

SH-form

Disulfide: [149287-05-8]. *2,2′-Dithiobis(1H-indole-3-acetic acid)*
$C_{20}H_{16}N_2O_4S_2$ M 412.4 Cryst. (CH_2Cl_2). Mp 208° (196-199°).

Disulfide, di-Me ester: [132637-90-2].
$C_{22}H_{20}N_2O_4S_2$ M 440.5 Cryst. (CH_2Cl_2/petrol). Mp 161-162°.

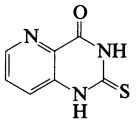
Disulfide, N,N′*-Di-Me:* [149287-06-9].
$C_{22}H_{20}N_2O_4S_2$ M 440.5 Cryst. (Me_2CO/petrol). Mp 190-192.5°.

Wieland, T. *et al, Annalen*, 1954, **587**, 146 (*synth, uv*)
Thompson, A.M. *et al, J. Med. Chem.*, 1993, **36**, 2459 (*synth, pmr*)

2,3-Dihydro-2-thioxopyrido[3,2-*d*]pyrimidin-4(1*H*)-one D-1-00333

*2-Mercapto-4-hydroxypyrido[3,2-*d*]pyrimidine*

[37891-05-7]



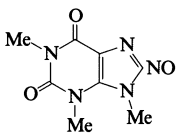
$C_7H_5N_3OS$ M 179.2
Cryst. (H_2O). Mp 300°.

Stanovnik, B. *et al, Synthesis*, 1972, 308.

3,9-Dihydro-1,3,9-trimethyl-8-nitroso-1*H*-purine-2,6-dione, 9CI D-1-00334

1,3,9-Trimethyl-8-nitrosoisoxanthine

[153534-80-6]



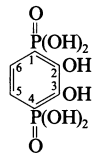
$C_8H_9N_5O_3$ M 223.1
The first isoxanthine (isocaffeine) deriv. from a natural source. Isol. from the sea cucumber *Cucumaria frondosa*. Powder. Mp 273° dec.

Yayli, N. *et al, J. Nat. Prod.*, 1994, **57**, 84 (*isol, uv, ir, pmr, cmr, struct*)

2,3-Dihydroxy-1,4-benzenediphosphonic acid D-1-00335

2,3-Dihydroxy-1,4-phenylenebisphosphonic acid. Hydroquinone-2,3-diphosphonic acid

[91633-18-0]



$C_6H_8O_8P_2$ M 270.0
Solid. Mp >300°.

Dianilinium salt: Cryst. Mp 211-213°.

Dhawan, B. *et al, J.O.C.*, 1984, **49**, 4018 (*synth, pmr, P-31 nmr*)

2,5-Dihydroxy-1,4-benzenediphosphonic acid D-1-00336

2,5-Dihydroxy-1,4-phenylenebisphosphonic acid. Hydroquinone-2,5-diphosphonic acid

[91633-16-8]

$C_6H_8O_8P_2$ M 270.0
Long needles (MeCN aq.). Mp 219-220°.

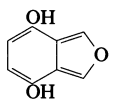
Tetra-Me ester: [88011-35-2]. *Tetramethyl 2,5-dihydroxy-1,4-phenylenebisphosphonate*
$C_{10}H_{16}O_8P_2$ M 326.1 Needles (Et_2O/petrol). Mp 126°.

Tetra-Et ester: [91633-15-7]. *Tetraethyl 2,5-dihydroxy-1,4-phenylenebisphosphonate. 2,5-Bis(diethoxyphosphinyl)-1,4-benzenediol. 2,5-Bis(diethoxyphosphinyl)hydroquinone*
$C_{14}H_{24}O_8P_2$ M 382.2 Cryst. (CH_2Cl_2/petrol). Mp 219-220°.

Trutmeva, E.K. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1983, 1684; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1983, 1532 (*tetra-Me ester, synth, ir, uv, pmr, P-31 nmr*)
Dhawan, B. *et al, J.O.C.*, 1984, **49**, 4018 (*synth, pmr, cmr, P-31 nmr*)
Nifant'ev, E.E. *et al, Zh. Obshch. Khim.*, 1992, **62**, 222; *J. Gen. Chem. USSR (Engl. Transl.)*, 1992, **62**, 186 (*pmr, P-31 nmr*)

4,7-Dihydroxybenzo[*c*]furan D-1-00337

Benzo[c]furan-4,7-diol



$C_8H_6O_3$ M 150.1

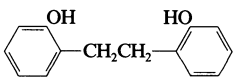
Di-Me ether: 4,7-Dimethoxybenzo[c]furan
$C_{10}H_{10}O_3$ M 178.1 Solid.

Lynch, V.M. *et al, Acta Cryst. C*, 1995, **51**, 780 (*synth, cryst struct, deriv*)

2,2′-Dihydroxybibenzyl D-1-00338

2,2′-(1,2-Ethanediyl)bisphenol, 9CI. 1,2-Bis(2-hydroxyphenyl)ethane

[29338-20-3]



$C_{14}H_{14}O_2$ M 214.2
Cryst. (H_2O). Mp 115°.

Di-Me ether: 1,2-Bis(2-methoxyphenyl)ethane
$C_{16}H_{18}O_2$ M 242.3 Cryst. (EtOH). Mp 86° (83-84°). Bp 290-300°.

Thiele, J. *et al, Annalen*, 1899, **305**, 99.
Irvine, J.C. *et al, J.C.S.*, 1907, **91**, 536.
Ross, J. *et al, Acta Cryst. C*, 1994, **50**, 976 (*cryst struct, di-Me ether*)

3,3′-Dihydroxybibenzyl D-1-00339

1,2-Bis(3-hydroxyphenyl)ethane. 3,3′-(1,2-Ethanediyl)bisphenol, 9CI

[70709-67-0]

$C_{14}H_{14}O_2$ M 214.2
Isol. from heartwood of *Cassia garrettiana* (Leguminosae) and *C. cortex*. Also isol. from the bark of *Cassia torosa* (Leguminosae). Needles (EtOAc/hexane, H_2O). Mp 139-140°.

Di-Me ether: 1,2-Bis(3-methoxyphenylethane)
$C_{16}H_{18}O_2$ M 242.3 Leaflets (EtOH). Mp 61-62° (39-40°). Bp_{10} 203°.

Cornforth, J.W. *et al, J.C.S.*, 1942, 684.
Hata, K. *et al, Chem. Pharm. Bull.*, 1979, **27**, 984 (*isol, synth*)

4,4′-Dihydroxybibenzyl D-1-00340

4,4′-(1,2-Ethanediyl)bisphenol, 9CI. 1,2-Bis(4-hydroxyphenyl)ethane

[6052-84-2]

$C_{14}H_{14}O_2$ M 214.2
Component for thermosetting resins. Needles (H_2O). Mp 184-186°, Mp 200°.

Mono-Me ether: 2-(4-Hydroxyphenyl)-1-(4-methoxyphenyl)ethane
$C_{15}H_{16}O_2$ M 228.2 Mp 113-115°.

Di-Me ether: 1,2-Bis(4-methoxyphenyl)ethane
$C_{16}H_{18}O_2$ M 242.3 Cryst. (EtOAc). Mp 118-120°, Mp 130°.

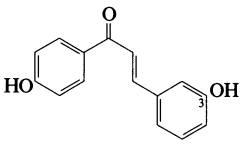
[52352-30-4, 63450-00-0, 133945-52-5, 133945-53-6]

Heumann, K. *et al, Ber.*, 1887, **20**, 909.
Buck, J.S. *et al, J.A.C.S.*, 1929, **51**, 2163 (*di-Me ether*)
Schiller, C.D. *et al, Arch. Pharm. (Weinheim, Ger.)*, 1990, **323**, 417 (*synth, pmr, mono-Me ether*)
Ungar, G. *et al, Macromolecules*, 1991, **24**, 1168 (*synth, pmr, di-Me ether*)

3,4′-Dihydroxychalcone D-1-00341

3-(3-Hydroxyphenyl)-1-(4-hydroxyphenyl)-2-propen-1-one, 9CI

[3654-50-0]



$C_{15}H_{12}O_3$ M 240.2
Mp 205-206°.

3-Me ether: [75849-15-9]. *3-Methoxy-4′-hydroxychalcone*
$C_{16}H_{14}O_3$ M 254.2 Yellow cryst. (EtOH aq.). Mp 138-141°.

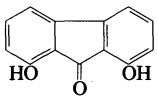
Di-Me ether: [52182-14-6]. *3,4′-Dimethoxychalcone*
$C_{17}H_{16}O_3$ M 268.3 Yellow leaflets (MeOH). Mp 96-97°.

Hudson, B.J.F., *J.C.S.*, 1946, 754 (*synth*)
Jurd, L. *et al, J.O.C.*, 1961, **26**, 2561 (*uv*)

Hahn, V. *et al, C. R. Hebd. Seances Acad. Sci.*, 1963, **257**, 1948 (*uv*)
Schwarz, M.A. *et al, J.A.C.S.*, 1977, **99**, 2571 (*di-Me ether*)
Murphy, W.S. *et al, J.C.S. Perkin 1*, 1980, 1567 (*3-Me ether*)
Gao, C. *et al, Synth. Commun.*, 1995, **25**, 1877 (*synth, pmr*)

1,8-Dihydroxy-9*H*-fluoren-9-one D-1-00342

[127375-30-8]



$C_{13}H_8O_3$ M 212.2
Yellow needles ($CHCl_3$). Mp 188-190°, Mp 238-240°.

Di-Me ether: [127375-31-9]. *1,8-Dimethoxy-9H-fluoren-9-one*
$C_{15}H_{12}O_3$ M 240.2 Yellow needles ($CHCl_3$). Mp 234-237°.

Shoji, K. *et al, Nippon Kagaku Kaishi*, 1989, 2046; *CA*, **112**, 234934r (*synth, ir, pmr*)
Sharma, V. *et al, J.O.C.*, 1994, **59**, 7785 (*synth, di-Me ether, ir, pmr, cmr*)

8,16-Dihydroxyhexadecanoic acid D-1-00343

[53950-52-0]

$HOH_2C(CH_2)_7CH(OH)(CH_2)_6COOH$

$C_{16}H_{32}O_4$ M 288.4
(+)-*form* [69079-56-7]
Constit. of various plant cutins.

Me ester: [109008-12-0]. ***Nerifol***
$C_{17}H_{34}O_4$ M 302.4 Constit. of the leaves of *Nerium odorum*. Needles (petrol). Mp 74-75°.

Me ester, di-Ac:
$C_{21}H_{38}O_6$ M 386.5 Needles (EtOAc). Mp 58-60°.

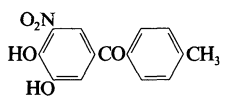
[77441-75-9]

Espelie, K.E. *et al, Lipids*, 1978, **13**, 832 (*occur*)
Tulloch, A.P. *et al, Lipids*, 1980, **15**, 881 (*synth, ms*)
Siddiqui, S. *et al, Planta Med.*, 1987, **53**, 47 (*Nerifol*)
Gerard, H.C. *et al, Phytochemistry*, 1994, **35**, 818 (*isol*)

3,4-Dihydroxy-4'-methyl-5-nitrobenzophenone D-1-00344

(3,4-Dihydroxy-5-nitrophenyl)(4-methylphenyl) methanone, 9CI. ***Tolcapone, INN, USAN.*** *Ro 40-7592*

[134308-13-7]

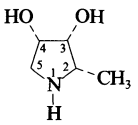


$C_{14}H_{11}NO_5$ M 273.2
Catechol-*O*-methyltransferase inhibitor. Used in combination therapy with 2-Amino-3-(3,4-dihydroxyphenyl)propanoic acid, A-0-01830 in treatment of Parkinson's disease. Yellow cryst. Mp 144-145°.
▶ LD_{50} (mus, orl) 1600 mg/kg. PC4952500.

Australian Pat., 603 788, (1990) (*Hoffmann-La Roche*); *CA*, **115**, 49134d (*synth, pharmacol*)
Da Prada, M. *et al, Adv. Behav. Biol.*, 1991, **39**, 723 (*pharmacol*)
Drugs of the Future, 1991, **16**, 719 (*rev*)
Mannisto, P.T. *et al, Br. J. Pharmacol.*, 1992, **105**, 569 (*pharmacol*)
Acquas, E. *et al, J. Neurochem.*, 1992, **59**, 326 (*metab*)
Tornwall, M. *et al, Eur. J. Pharmacol.*, 1993, **239**, 39 (*pharmacol*)
Friedgen, B. *et al, Naunyn-Schmiedeberg's Arch. Pharmacol.*, 1993, **347**, 155 (*pharmacol*)
Kaakkola, S. *et al, Gen. Pharmacol.*, 1994, **25**, 813 (*rev*)
Napolitano, A. *et al, Eur. J. Pharmacol.*, 1995, **273**, 215 (*pharmacol*)

3,4-Dihydroxy-2-methylpyrrolidine D-1-00345

2-Methyl-3,4-pyrrolidinediol, 9CI

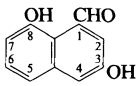


$C_5H_{11}NO_2$ M 117.1
(2S,3R,4S)-form [162895-59-2]
Oil. $[\alpha]_D^{25}$ +20.5 (c, 0.65 in D_2O).

[162600-04-6]

Wong, C.-H. *et al, J.O.C.*, 1995, **60**, 1492 (*synth, pmr, cmr*)

3,8-Dihydroxy-1-naphthalenecarboxaldehyde D-1-00346



$C_{11}H_8O_3$ M 188.1
Solid (toluene). Mp 230-231°.

Saá, J.M. *et al, J.A.C.S.*, 1995, **117**, 1105 (*synth, pmr, cmr*)

5,8-Dihydroxy-1-naphthalenecarboxaldehyde D-1-00347

$C_{11}H_8O_3$ M 188.1
Red solid (cyclohexane). Mp 182-185°.

Saá, J.M. *et al, J.A.C.S.*, 1995, **117**, 1105 (*synth, pmr, cmr*)

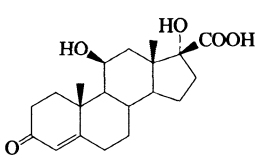
6,8-Dihydroxy-1-naphthalenecarboxaldehyde D-1-00348

$C_{11}H_8O_3$ M 188.1
Yellow solid (toluene). Mp 151-153°.

Saá, J.M. *et al, J.A.C.S.*, 1995, **117**, 1105 (*synth, pmr, cmr*)

11,17-Dihydroxy-3-oxo-4-androstene-17-carboxylic acid D-1-00349

11,17-Dihydroxy-3-oxo-4-etiocholenic acid. 11,17-Dihydroxy-3-keto-Δ^4-17-isoetienic acid



$C_{20}H_{28}O_5$ M 348.4
(11β,17α)-form [3597-45-3]
Cortienic acid
Inactive metab. of 11,17,21-Trihydroxypregn-4-ene-3,20-dione, T-0-05318. Cryst. (EtOAc). Mp 240-244° (230-232°).

Me ester: [10486-88-1].
$C_{21}H_{30}O_5$ M 362.4 Cryst. (EtOAc/Et_2O). Mp 206-207° (192-194°). $[\alpha]_D$ +121 (EtOH).
(11β,17β)-form [100188-36-1]
Cryst. + $\frac{1}{2}$ H_2O (EtOAc). Mp 201-203°. $[\alpha]_D^{29}$ +116 (EtOH).

Me ester: Cryst. Mp 204-206°.

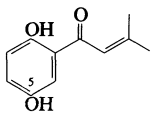
[7323-94-6, 85617-72-7]

Woodward, R.B. *et al, J.A.C.S.*, 1952, **74**, 4223 (*synth*)
Caspi, E. *et al, Tetrahedron*, 1961, **16**, 271 (*synth*)
Zuercher, R.F. *et al, Helv. Chim. Acta*, 1963, **46**, 2054 (*pmr*)
Georgian, V. *et al, Tetrahedron*, 1963, **19**, 1037 (*synth*)
Druzgala, P. *et al, Synth. Commun.*, 1990, **20**, 1133 (*synth*)

1-(2,5-Dihydroxyphenyl)-3-methyl-2-buten-1-one D-1-00350

2-(3-Methyl-2-butenoyl)-1,4-benzenediol. β,β-Dimethacryloxylhydroquinone. 2',5'-Dihydroxy-3-methylcrotonophenone. 2-Senecioylhydroquinone

[150692-98-1]



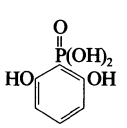
$C_{11}H_{12}O_3$ M 192.2
Isol. from the leaf resin of *Nama* sp. Dark yellow solid.

5-Me ether: [84346-78-1]. *1-(2-Hydroxy-5-methoxyphenyl)-3-methyl-2-buten-1-one, 9CI*
$C_{12}H_{14}O_3$ M 206.2 Isol. from *Calea prunifolia*. Mp 48-49°.

Di-Me ether: [121637-62-5]. *1-(2,5-Dimethoxyphenyl)-3-methyl-2-buten-1-one, 9CI*
$C_{13}H_{16}O_3$ M 220.2 Bp_5 165-168°.

Camps, F. *et al, J. Het. Chem.*, 1985, **22**, 363 (*synth, deriv*)
Ramana, M.M.V. *et al, Indian J. Chem., Sect. B*, 1988, **27**, 339 (*di-Me ether*)
Castro, V. *et al, Phytochemistry*, 1989, **28**, 2415 (*isol, deriv*)
Roitman, J.N. *et al, Phytochemistry*, 1993, **33**, 936 (*isol, pmr, cmr*)

2,6-Dihydroxyphenylphosphonic acid D-1-00351



$C_6H_7O_5P$ M 190.0
Mono-Me ether: [136829-81-7]. *(2-Hydroxy-6-methoxyphenyl)phosphonic acid*
$C_7H_9O_5P$ M 204.1 Cryst. (CH_2Cl_2). Mp 113-119°.

Mono-Me ether, Di-Et ester: Diethyl (*2-hydroxy-6-methoxyphenyl*)phosphonate
$C_{11}H_{17}O_5P$ M 260.2 Liq. $Bp_{0.04}$ 118-122°.

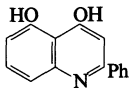
Mono-Me ether, bis(2-methylpropyl) ester: [129529-32-4]. *Bis(2-methylpropyl) (2-hydroxy-6-methoxyphenyl)phosphonate*
$C_{15}H_{25}O_5P$ M 316.3 Liq. $Bp_{0.1}$ 106-108°.

*Mono-Me ether, di-*tert*-butyl ester:* [136829-79-3]. *Bis(1,1-dimethylethyl) (2-hydroxy-6-methoxyphenyl)phosphonate*
$C_{15}H_{25}O_5P$ M 316.3 Cryst. (petrol). Mp 80-81°.

Melvin, L.S., *Tet. Lett.*, 1981, **22**, 3375 (*di-Et ester*)
Li, S. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1990, **48**, 251; 1991, **61**, 119 (*diisobutyl ester, synth, ir, ms, pmr, P-31 nmr*)
Dhawan, B. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **61**, 183 (*synth, di-tert-butyl ester, pmr, cmr, P-31 nmr*)

4,5-Dihydroxy-2-phenylquinoline D-1-00352

5-Hydroxy-2-phenyl-4(1H)-quinolinone, 9CI
2-Phenyl-4,5-quinolinediol



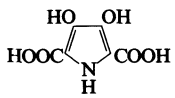
$C_{15}H_{11}NO_2$ M 237.2

NH-form

N-*Me:* [19843-07-3]. *5-Hydroxy-1-methyl-2-phenyl-4(1H)-quinolinone*
$C_{16}H_{13}NO_2$ M 251.2 Minor alkaloid from leaves of *Lunasia quercifolia* (Rutaceae). Pale yellow needles (MeOH). Mp 174-176°.

Hart, N.K. *et al*, *Aust. J. Chem.*, 1968, **21**, 1389 (*isol, pmr, ms, struct*)
Venturella, P. *et al*, *Gazz. Chim. Ital.*, 1970, **100**, 678 (*synth*)

3,4-Dihydroxy-1*H*-pyrrole-2,5-dicarboxylic acid D-1-00353



$C_6H_5O_6$ M 173.1

Di-Me ester: [1632-19-5].
$C_8H_9O_6$ M 201.1 Cryst. (MeOH); yellow powder (H_2O). Mp 217-218° (207°).

Di-Me ether: [157283-08-4]. *3,4-Dimethoxy-1H-pyrrole-2,5-dicarboxylic acid, 9CI*
$C_8H_9O_6$ M 201.1 Cryst. (MeCN). Mp 180° dec.

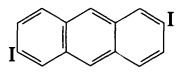
Di-Me ether, Di-Me ester: [1632-57-1].
$C_{10}H_{13}O_6$ M 229.2 Cryst. (Et_2O). Mp 84-86° (75°).

Di-Et ether: 3,4-Diethoxy-1H-pyrrole-2,5-dicarboxylic acid
$C_{12}H_{13}O_6$ M 253.2 Powder. Mp 170° dec.

Wåhlstam, H., *Ark. Kemi*, 1957, **11**, 251 (*di-Me ester*)
Friedman, M., *J.O.C.*, 1965, **30**, 859 (*di-Me ester, di-Me ether*)
Merz, A. *et al*, *Synthesis*, 1995, 795 (*ester, di-Me ether*)

2,6-Diiodoanthracene D-1-00354

[148239-77-4]

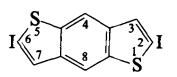


$C_{14}H_8I_2$ M 430.0

Yanagimoto, T. *et al*, *Chem. Comm.*, 1993, 519 (*synth*)

2,6-Diiodobenzo[1,2-*b*:4,5-*b'*]dithiophene, 9CI D-1-00355

[155904-20-4]

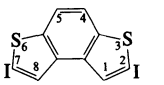


$C_{10}H_4I_2S_2$ M 442.0
Leaflets (chlorobenzene). Mp >300°.

Yoshida, S. *et al*, *J.O.C.*, 1994, **59**, 3077 (*synth, pmr*)

2,7-Diiodobenzo[1,2-*b*:4,3-*b'*]dithiophene, 9CI D-1-00356

[70218-29-0]

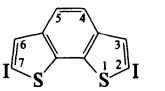


$C_{10}H_4I_2S_2$ M 442.0
Needles (C_6H_6/hexane). Mp 175-176°.

Gronowitz, S. *et al*, *Chem. Scr.*, 1977, **12**, 97 (*synth, pmr, cmr*)
Yoshida, S. *et al*, *J.O.C.*, 1994, **59**, 3077 (*synth, pmr, cmr*)

2,7-Diiodobenzo[2,1-*b*:3,4-*b'*]dithiophene, 9CI D-1-00357

[156355-43-0]

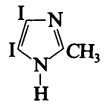


$C_{10}H_4I_2S_2$ M 442.0
Needles (C_6H_6). Mp 186-188°.

Yoshida, S. *et al*, *J.O.C.*, 1994, **59**, 3077 (*synth, pmr, cmr*)

4,5-Diiodo-2-methylimidazole, 9CI D-1-00358

[73746-44-8]



$C_4H_4I_2N_2$ M 333.8
Cryst. (H_2O). Mp 204-206° dec. (194-195°).

1H-form

1-Me: [13369-82-9]. *4,5-Diiodo-1,2-dimethyl-1H-imidazole*
$C_5H_6I_2N_2$ M 347.9 Prisms (EtOAc). Mp 142°.

Vaughan, J.D. *et al*, *J.O.C.*, 1980, **45**, 3108 (*synth*)
Pyne, S.G. *et al*, *Synthesis*, 1994, 681 (*synth, ir, pmr, ms*)

3,4-Diiodopyrazole D-1-00359

[6645-70-1]

$C_3H_2I_2N_2$ M 319.8
Needles (C_6H_6). Mp 160-162° (159-160°).

N-*Ac:*
$C_5H_4I_2N_2O$ M 361.9 Cryst. (petrol). Mp 83-85°.

N-*Benzoyl:*
$C_{10}H_6I_2N_2O$ M 423.9 Cryst. Mp 107-109°.

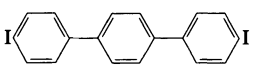
N-(*4-Methylbenzenesulfonyl*): Cryst. Mp 130-131°.

N-*Benzyl:*
$C_{10}H_8I_2N_2$ M 409.9 Cryst. Mp 63-66°.

Giles, D. *et al*, *J.C.S.(C)*, 1966, 1179 (*synth*)
Holzer, W. *et al*, *J. Het. Chem.*, 1995, **32**, 189 (*derivs*)

4,4″-Diiodo-1,1′:4′,1″-terphenyl, 9CI D-1-00360

[19053-14-6]



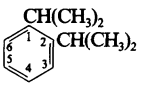
$C_{18}H_{12}I_2$ M 482.1
Scales (toluene). Mp 327-328° (307-309° dec.).

Kovyrzina, K.A. *et al*, *Zh. Org. Khim.*, 1974, **10**, 1067; *J. Org. Chem. USSR (Engl. Transl.)*, 1974, **10**, 1078 (*synth*)
Unroe, M.R. *et al*, *Synthesis*, 1987, 981 (*synth*)
Zauhar, J. *et al*, *Synthesis*, 1995, 703 (*synth, ir*)

1,2-Diisopropylbenzene, 8CI D-1-00361

1,2-Bis(1-methylethyl)benzene, 9CI

[577-55-9]



$C_{12}H_{18}$ M 162.2
Liq. Bp 203.8°.

Melpolder, F.W. *et al*, *J.A.C.S.*, 1948, **70**, 935 (*synth, ir, uv, ms*)
Adv. Chem. Ser., 1955, **15**, 99 (***props***)
Elsner, B.B. *et al*, *J.C.S.*, 1957, 578 (*synth*)

1,3-Diisopropylbenzene, 8CI D-1-00362

1,3-Bis(1-methylethyl)benzene, 9CI

[99-62-7]

$C_{12}H_{18}$ M 162.2
Liq. Bp 203.2°.

Newton, A., *J.A.C.S.*, 1943, **65**, 320 (*synth*)
Melpolder, F.W. *et al*, *J.A.C.S.*, 1948, **70**, 935 (*synth, ir, uv, ms*)
Adv. Chem. Ser., 1955, **15**, 100 (***props***)
Sudmeijer, O. *et al*, *Org. Magn. Reson.*, 1984, **22**, 459 (*cmr*)

1,4-Diisopropylbenzene, 8CI D-1-00363

1,4-Bis(1-methylethyl)benzene, 9CI

[100-18-5]

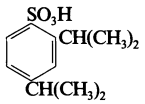
$C_{12}H_{18}$ M 162.2
Liq. Bp 210.4°.

Newton, A., *J.A.C.S.*, 1943, **65**, 320 (*synth*)
Melpolder, F.W. *et al*, *J.A.C.S.*, 1948, **70**, 935 (*synth, ir, uv, ms*)
Adv. Chem. Ser., 1955, **15**, 101 (***props***)
Zavgorodnii, S.V. *et al*, *Zh. Obshch. Khim.*, 1958, **28**, 1279; *CA*, **52**, 20015f (*synth*)
Kravers, M.A. *et al*, *Cryst. Struct. Commun.*, 1979, **8**, 455 (*cryst struct*)
Sudmeijer, O. *et al*, *Org. Magn. Reson.*, 1984, **22**, 459 (*cmr*)

2,4-Diisopropylbenzenesulfonic acid D-1-00364

2,4-Bis(1-methylethyl)benzenesulfonic acid

[63877-48-5]



$C_{12}H_{18}O_3S$ M 242.3

Chloride: [93777-28-7].
$C_{12}H_{17}ClO_2S$ M 260.7 Mp 37-38°.

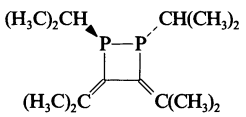
Amide:
$C_{12}H_{19}NO_2S$ M 241.3 Mp 144-145°.

Anilide:
$C_{18}H_{23}NO_2S$ M 317.4 Mp 113.9-114.5°.

Newton, A. *et al*, *J.A.C.S.*, 1943, **65**, 2439.
Cerfontain, H. *et al*, *J.C.S. Perkin 2*, 1977, 717.

1,2-Diisopropyl-3,4-diisopropylidene-1,2-diphosphetane D-1-00365

1,2-Bis(1-methylethyl)-3,4-bis(1-methylethylidene)-1,2-diphosphetane, 9CI



$C_{14}H_{26}P_2$ M 256.3

(1RS,2RS)-form
(±)-trans-*form*
Solid. Mp 36-38°.

Disulfide:
$C_{14}H_{26}P_2S_2$ M 320.4 Cryst. (hexane). Mp 130-132°.

[149206-08-6, 149206-09-7]

Brieden, W. *et al*, *Chem. Ber.*, 1993, **126**, 845 (*synth, ir, ms, pmr, cmr, P-31 nmr, cryst struct*)

Diisopropyl selenide D-1-00366

2,2'-Selenobispropane, 9CI

[37773-02-7]

$(H_3C)_2CHSeCH(CH_3)_2$

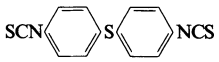
$C_6H_{14}Se$ M 165.1
Bp 136-137°.

Odom, J.D. *et al*, *J.A.C.S.*, 1979, **101**, 5815.

4,4'-Diisothiocyanatodiphenyl sulfide D-1-00367

1,1'-Thiobis[4-isothiocyanatobenzene], 9CI

[15398-68-2]



$C_{14}H_8N_2S_3$ M 300.4

S,S-*Dioxide:* [4430-49-3]. *1,1'-Sulfonylbis[4-isothiocyanatobenzene], 9CI.* ***Centsulphone***
$C_{14}H_8N_2O_2S_3$ M 332.4 Anthelmintic. Mp 180° (169°).

Saxena, R. *et al*, *Indian J. Pharm.*, 1967, **29**, 232 (*synth, props*)
Katiyar, J.C. *et al*, *Nature (London)*, 1967, **214**, 708 (*props*)
Uher, M. *et al*, *Coll. Czech. Chem. Comm.*, 1969, **34**, 4005 (*uv, struct*)
Sharma, S. *et al*, *Indian J. Pharm.*, 1973, **35**, 13 (*synth, props*)

3,3-Dimethoxy-2-propenenitrile D-1-00368

3,3-Dimethoxyacrylonitrile. 2-Cyano-1,1-dimethoxyethylene

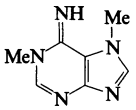
$(MeO)_2C{=}CHCN$

$C_5H_7NO_2$ M 113.1
Intermed. for isoxazoles. Syrup. Bp_{19} 112-115°.

Tatsuta, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1994, **67**, 1701.

1,7-Dimethyladenine D-1-00369

1,7-Dihydro-1,7-dimethyl-6H-purin-6-imine



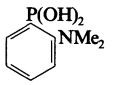
$C_7H_9N_5$ M 163.1
Hygroscopic solid. Mp 164-165°.

Hydrochloride: Hygroscopic solid. Mp 224.5-230° dec.

Perchlorate: Needles. Mp 278-280° dec.

Fujii, T. *et al*, *Chem. Pharm. Bull.*, 1993, **41**, 2047; 1994, **42**, 151 (*synth, uv, pmr*)

[2-(Dimethylamino)phenyl] phosphonous acid D-1-00370



$C_8H_{12}NO_2P$ M 185.1

Difluoride: [110538-89-1].
$C_8H_{10}F_2NP$ M 189.1 Ligand for Pt. Liq. Bp_2 63-66°.

Dichloride: [110538-87-9].
$C_8H_{10}Cl_2NP$ M 222.0 Liq. $Bp_{0.1}$ 71°.

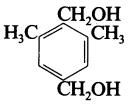
Bis(diethylamide): [110538-86-8].
$C_{16}H_{30}N_3P$ M 295.4 Liq. Bp_1 138-140°.

Heuer, L. *et al*, *Polyhedron*, 1987, **6**, 1295 (*synth, pmr, P-31 nmr, F-19 nmr*)
Heuer, L. *et al*, *J. Fluorine Chem.*, 1988, **39**, 197 (*difluoride, F-19 nmr, P-31 nmr, complex*)

2,6-Dimethyl-1,4-benzenedimethanol D-1-00371

1,4-Bis(hydroxymethyl)-2,6-dimethylbenzene

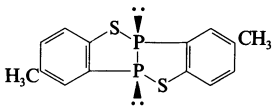
[157248-87-8]



$C_{10}H_{14}O_2$ M 166.2
Cryst. (cyclohexane). Mp 143-145°.

Lai, Y.-H. *et al*, *J.O.C.*, 1994, **59**, 3381 (*synth, pmr, ir, ms*)

2,8-Dimethyl[1,2,3]benzothiadiphospholo[3,2-*b*][1,2,3]benzothiodiphosphole D-1-00372



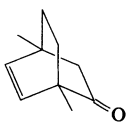
$C_{14}H_{12}P_2S_2$ M 306.3

(6RS,12SR)-form
(±)-cis-*form*
Possesses a 'butterfly' struct. Yellow flattened prisms.

Baccolini, G. *et al*, *Heteroat. Chem.*, 1993, **4**, 319 (*synth, ms, pmr, cmr, P-31 nmr, cryst struct*)

1,4-Dimethylbicyclo[2.2.2]oct-5-en-2-one, 9CI D-1-00373

[156140-50-0]

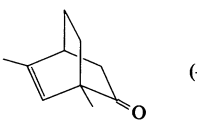


$C_{10}H_{14}O$ M 150.2

(±)-***form*** [89398-35-6]
Oil. Bp_{10} 68-70°.

Snowden, R.L. *et al*, *Helv. Chim. Acta*, 1989, **72**, 570 (*synth, ir, pmr, cmr, ms*)
Zhang, W. *et al*, *Tetrahedron*, 1993, **49**, 1965 (*synth*)

1,5-Dimethylbicyclo[2.2.2]oct-5-en-2-one, 9CI D-1-00374



(–)-*form*

$C_{10}H_{14}O$ M 150.2

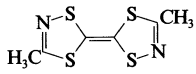
(–)-***form***
Liq. Bp_{23} 103-105°. $[\alpha]_D^{18}$ –443 (c, 1.3 in $CHCl_3$). n_D^{18} 1.4868.

[123004-30-8]

Mori, K. *et al*, *Synthesis*, 1995, 845 (*synth, pmr*)

3,3′-Dimethylbi(1,4,2-dithiazol-5-ylidene) D-1-00375

3-Methyl-5-(3-methyl-1,4,2-dithiazol-5-ylidene)-1,4,2-dithiazole, 9CI



(E)-form

$C_6H_6N_2S_4$ M 234.3

(E)-form [152597-07-4]
Cryst. Mp 146-148°.

(Z)-form [151451-86-4]
Cryst. Mp 114°.

Oakley, R.T. *et al*, *Chem. Comm.*, 1993, 1226 (*synth, cryst struct*)

1,1-Dimethyl-2,2-bis(trifluoromethyl) diphosphine, 9CI D-1-00376

[666-62-6]

$Me_2P—P(CF_3)_2$

$C_4H_6F_6P_2$ M 230.0
Ligand for W, Cr and Mo carbonyls. Liq. Mp −79.2° to −79.1°. Bp 120° (est.). V.p. 4.94 mm at 0°, 55.1 mm at 45.1°. Dec. at 110°.

BH_3 (1:1) adduct:
$C_4H_9BF_6P_2$ M 243.8 Mp −30.2 to −29.6°. Dec. at 90°→$(CF_3)_2PH$.

Me_3N (1:1) adduct:
$C_7H_{15}F_6NP_2$ M 289.1 Yellow oil.

Monomethiodide:
$C_5H_9F_6IP_2$ M 371.9 Solid. Subl. 200°. Struct. not known.

Grant, L.R. *et al*, *J.A.C.S.*, 1962, **84**, 1834 (*synth, uv, props, derivs*)
Cavell, R.G. *et al*, *J.C.S.(A)*, 1968, 1406 (*synth, ms, ir, pmr, F-19 nmr, P-31 nmr*)
Cowley, A.H. *et al*, *J.A.C.S.*, 1974, **96**, 3666 (*pe*)
Grobe, J. *et al*, *Z. Naturforsch., B*, 1979, **34**, 1653; 1980, **35**, 694 (*complexes, ms, ir, pmr, F-19 nmr, P-31 nmr*)
Grobe, J. *et al*, *Z. Anorg. Allg. Chem.*, 1984, **518**, 36 (*cmr, P-31 nmr, complexes*)
Avens, L.R. *et al*, *Inorg. Chem.*, 1989, **28**, 211 (*synth, F-19 nmr, P-31 nmr*)

1,2-Dimethyl-1,2-bis(trifluoromethyl) diphosphine D-1-00377

[4669-75-4]

$F_3CPMe—PMeCF_3$

$C_4H_6F_6P_2$ M 230.0
Obt. only as steroisomeric mixt. V.p. 4.0 mm at 0°, 30.6 mm at 35°.

[33418-05-2, 33418-06-3]

Burg, A.B. *et al*, *J.A.C.S.*, 1966, **88**, 31 (*synth, ir, props*)
Kang, D. *et al*, *Org. Magn. Reson.*, 1971, **3**, 101 (*pmr, F-19 nmr, P-31 nmr*)
Dobbie, R.C. *et al*, *Chem. Comm.*, 1975, 585 (*synth*)
Grobe, J., *Z. Naturforsch., B*, 1988, **43**, 427 (*synth, pmr, F-19 nmr, P-31 nmr*)

2,2-Dimethyl-1,4-butanediol, 9CI D-1-00378

[32812-23-0]

$HOH_2CCH_2C(CH_3)_2CH_2OH$

$C_6H_{14}O_2$ M 118.1
Liq. Bp 229-233°, Bp_8 110°.

Bis-4-methylbenzenesulfonyl: [67857-74-3]. Cryst. Mp 84-85° (77-78°).

Bouveault, L. *et al*, *Bull. Soc. Chim. Fr.*, 1904, **31**, 1203 (*synth*)
Brown, R.F. *et al*, *J.A.C.S.*, 1955, **77**, 1089 (*synth*)
Derbesy, M. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 1789 (*synth*)
Fitjer, L. *et al*, *Synthesis*, 1994, 893 (*synth, deriv*)

(3,3-Dimethyl-1-butynyl) phosphonic acid, 9CI D-1-00379

tert-*Butylacetylenephosphonic acid*

$(H_3C)_3CC{\equiv}CP(O)(OH)_2$

$C_6H_{11}O_3P$ M 162.1

Di-Et ester: [40632-91-5]. *Diethyl (3,3-dimethyl-1-butynyl)phosphonate*
$C_{10}H_{19}O_3P$ M 218.2 Liq. d_4^{20} 0.93. Bp_1 107°. n_D^{20} 1.4706; n_D^{20} 1.4416.

Diisopropyl ester: [125172-82-9]. *Diisopropyl (3,3-dimethyl-1-butynyl)phosphonate*
$C_{12}H_{23}O_3P$ M 246.2 Liq.

Dichloride: [40632-82-4].
$C_6H_9Cl_2OP$ M 199.0 Solid or liq. Mp 32-34°. Bp_1 53-55°.

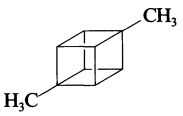
[125172-81-8]

Dogadina, A.V. *et al*, *Zh. Obshch. Khim.*, 1972, **42**, 2186; *J. Gen. Chem. USSR (Engl. Transl.)*, 1972, **42**, 2183 (*dichloride, diethyl ester, synth, pmr*)
Haegele, G. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1990, **48**, 131 (*esters, synth, pmr, P-31 nmr*)

1,4-Dimethylcubane D-1-00380

1,4-Dimethylpentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane, 9CI

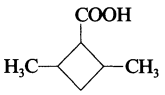
[161088-18-2]



$C_{10}H_{12}$ M 132.2
Needles. Mp 41-42°.

Eaton, P.E. *et al*, *J.O.C.*, 1995, **60**, 966 (*synth, pmr, cmr*)

2,4-Dimethylcyclobutanecarboxylic acid D-1-00381



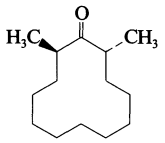
$C_7H_{12}O_2$ M 128.1
Liq. Obt. as a mixt. of isomers separated by glc.

[149193-25-9, 149251-10-5]

Török, B. *et al*, *J.C.S. Perkin 1*, 1993, 801 (*synth, ms, pmr*)

2,12-Dimethylcyclododecanone D-1-00382

[32399-58-9]



(2RS,12RS)-form

$C_{14}H_{26}O$ M 210.3
Both stereoisomers known, no phys. props. reported.

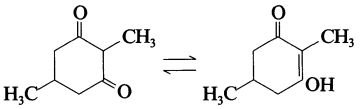
[86195-63-3, 86195-64-4]

Posner, G.H. *et al*, *J.A.C.S.*, 1973, **95**, 3076.
Vedejs, E. *et al*, *J.A.C.S.*, 1983, **105**, 5058.

2,5-Dimethyl-1,3-cyclohexanedione, 9CI D-1-00383

3-Hydroxy-2,5-dimethyl-2-cyclohexen-1-one

[61621-47-4]

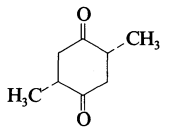


$C_8H_{10}O_2$ M 138.1
Needles or prisms (H_2O). Mp 175-176°.

Sonn, A., *Ber.*, 1931, **64**, 1847 (*synth*)
Stetter, H. *et al*, *Chem. Ber.*, 1957, **90**, 2928 (*synth*)
Leed, A.R. *et al*, *J.O.C.*, 1980, **45**, 1098 (*synth, pmr*)
Majetich, G. *et al*, *J.O.C.*, 1988, **53**, 50 (*synth, pmr, ir*)
Joseph, D. *et al*, *Org. Prep. Proced. Int.*, 1995, **27**, 499 (*synth, pmr*)

2,5-Dimethyl-1,4-cyclohexanedione, 9CI D-1-00384

[583-81-3]



(2RS,5RS)-form

$C_8H_{12}O_2$ M 140.1

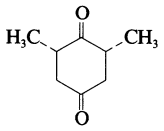
(2RS,5RS)-form [43126-02-9]
(±)-cis-*form*
Needles (petrol). Mp 118-118.5°.

(2RS,5SR)-form [43126-07-4]
trans-*form*
Needles. Mp 93° (85-87°).

Baeyer, A., *Ber.*, 1892, **25**, 2122 (*synth*)
Fishman, J. *et al*, *J.C.S.*, 1960, 3948 (*synth*)
Stolow, R.D. *et al*, *Tet. Lett.*, 1964, 95 (*conformn*)
Corey, E.J. *et al*, *Chem. Ber.*, 1978, **111**, 1337 (*synth, ir, pmr*)
Andersen, J.R. *et al*, *J.C.S. Perkin 1*, 1979, 3095 (*synth, pmr, ms*)
Queiroz, M.-J. *et al*, *Org. Prep. Proced. Int.*, 1995, **27**, 120 (*synth, pmr, cmr, ms*)

2,6-Dimethyl-1,4-cyclohexanedione, 9CI D-1-00385

[14384-30-6]



$C_8H_{12}O_2$ M 140.1

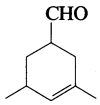
(2RS,6SR)-form [34958-43-5]
cis-*form*
Cryst. (hexane). Mp 87.5-88°.

Teuber, H.-J. *et al*, *Annalen*, 1966, **696**, 116 (*synth*)
Stolow, R.D. *et al*, *J.O.C.*, 1972, **37**, 2894 (*synth*)

3,5-Dimethyl-3-cyclohexene-1-carboxaldehyde, 9CI, 8CI D-1-00386

Cyclal C

[68039-48-5]

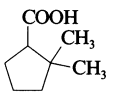


$C_9H_{14}O$ M 138.2
Important perfumery ingredient. Liq. with powerful leafy floral odour. d 0.92.

Japan. Pat., 5 901 462, (1984); *CA*, **101**, 6689g.
Japan. Pat., 61 65 801, (1986); *CA*, **105**, 74388r.

2,2-Dimethylcyclopentanecarboxylic acid D-1-00387

[63861-26-7]



$C_8H_{14}O_2$ M 142.1

(±)-*form*
Liq.

Me ester: [153579-98-7].
$C_9H_{16}O_2$ M 156.2 Liq. Bp_{25} 78°.

4-Bromophenacyl ester: [63861-28-9].
Needles (EtOH). Mp 55-57.7°.

Anilide:
$C_{14}H_{19}NO$ M 217.3 Cryst. Mp 125°.

Nitrile: [153580-00-8]. *2-Cyano-1,1-dimethylcyclopentane*
$C_8H_{13}N$ M 123.1 Pale yellow liq.

[63861-27-8]

Edwards, O.E. *et al*, *J.O.C.*, 1959, **24**, 2071 (*synth, ir, pmr*)
Kirk, D.N. *et al*, *J.C.S. Perkin 1*, 1977, 893 (*synth, pmr*)
Peterson, E.M. *et al*, *J. Med. Chem.*, 1994, **37**, 275 (*nitrile, Me ester, synth, ir, pmr, cmr*)

3,3-Dimethylcyclopentanecarboxylic acid D-1-00388

[69393-30-2]

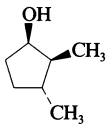
$C_8H_{14}O_2$ M 142.1

(±)-*form*
Liq. $Bp_{0.1}$ 63-65°.

Me ester: [69393-31-3].
$C_9H_{16}O_2$ M 156.2 Liq. Bp_{15} 65-70°.

Iwasaki, S. *et al*, *Helv. Chim. Acta*, 1978, **61**, 2831 (*synth, ir, pmr, ms*)

2,3-Dimethylcyclopentanol D-1-00389



(1*R*,2*S*,3*R*)-*form*

$C_7H_{14}O$ M 114.1

(1R,2S,3R)-form [153063-46-8]
$[\alpha]_D^{23}$ −61.3 (c, 1.1 in $CHCl_3$).

(1S,2R,3S)-form [153063-47-9]
$[\alpha]_D^{23}$ +49.4 (c, 1.4 in $CHCl_3$) (*ca.* 79% ee).

(1RS,2SR,3RS)-form [153063-45-7]
Liq. Bp_{30} 80-100° (Kugelrohr).

Chloroacetate: [153063-52-6].
$C_9H_{15}ClO_2$ M 190.6 Yellowish liq.

Varech, D. *et al*, *Bull. Soc. Chim. Fr.*, 1965, 1662 (*synth*)
Lora, M.D. *et al*, *J.O.C.*, 1995, **60**, 191 (*synth, ir, pmr, cmr*)

1,1-Dimethyl-2,2-diphenyldiphosphine, 9CI D-1-00390

[39654-12-1]

$Me_2P—PPh_2$

$C_{14}H_{16}P_2$ M 246.2
No phys. props. reported.

2-Sulfide: [73719-58-1].
$C_{14}H_{16}P_2S$ M 278.2 Formed preferentially (vs. 1-sulfide) and identified spectroscopically.

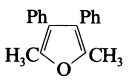
1,2-Disulfide: [31698-52-9].
$C_{14}H_{16}P_2S_2$ M 310.3 Cryst. (EtOH). Mp 145°.

[56912-73-3]

Koketsu, J. *et al*, *Inorg. Nucl. Chem. Lett.*, 1971, **7**, 15 (*disulfide*)
McFarlane, H.C.E. *et al*, *J.C.S. Dalton*, 1980, 240 (*synth, derivs, pmr, P-31 nmr*)

2,5-Dimethyl-3,4-diphenylfuran, 9CI D-1-00391

[63806-52-0]



$C_{18}H_{16}O$ M 248.3
Cryst. (MeOH). Mp 92°.

Hambrecht, J., *Synthesis*, 1977, 280 (*synth*)
Koenig, H. *et al*, *Annalen*, 1981, 668 (*synth*)
Bartmann, E. *et al*, *Synth. Commun.*, 1987, **17**, 263 (*synth*)

3,4-Dimethyl-2,5-diphenylfuran, 9CI D-1-00392

[51181-43-2]

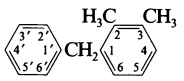
$C_{18}H_{16}O$ M 248.3
Mp 52-54°.

Inoue, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 2211 (*synth*)

2,3-Dimethyldiphenylmethane D-1-00393

1,2-Dimethyl-3-(phenylmethyl)benzene, 9CI. Phenyl-2,3-xylylmethane. 3-Benzyl-o-xylene. 1-Benzyl-2,3-dimethylbenzene

[62155-16-2]



$C_{15}H_{16}$ M 196.2
Liq. Bp_{33} 123°.

Tashiro, M. *et al*, *J.O.C.*, 1978, **43**, 1413 (*synth, ir, pmr*)
Fujiwara, J. *et al*, *Bull. Chem. Soc. Jpn.*, 1993, **66**, 1258 (*pmr, ms*)

2,4-Dimethyldiphenylmethane D-1-00394

*2,4-Dimethyl-1-(phenylmethyl)benzene, 9CI. Phenyl-2,4-xylylmethane. 4-Benzyl-*m*-xylene*

[28122-28-3]

$C_{15}H_{16}$ M 196.2
Oil. $Bp_{1.2}$ 139-142°. n_D^{22} 1.5678.

Clar, E. *et al*, *Ber.*, 1931, **64**, 981 (*synth*)
Errede, L.A. *et al*, *J.A.C.S.*, 1960, **82**, 3653 (*synth, ir, pmr*)
Mincione, E. *et al*, *Gazz. Chim. Ital.*, 1982, **112**, 437 (*pmr*)

2,5-Dimethyldiphenylmethane D-1-00395

*1,4-Dimethyl-2-(phenylmethyl)benzene, 9CI. Phenyl-2,5-xylylmethane, 8CI. 2-Benzyl-*p*-xylene*

[13540-50-6]

$C_{15}H_{16}$ M 196.2
$Bp_{1.5}$ 127-128°. n_D^{22} 1.5697.

Errede, L.A. *et al*, *J.A.C.S.*, 1960, **82**, 3653 (*synth, pmr, ir*)
Mathew, F. *et al*, *Synth. Commun.*, 1995, **25**, 1795 (*pmr, ir*)

2,6-Dimethyldiphenylmethane D-1-00396

*1,3-Dimethyl-2-(phenylmethyl)benzene, 9CI. Phenyl-2,6-xylylmethane, 8CI. 2-Benzyl-*m*-xylene*

[28122-29-4]

$C_{15}H_{16}$ M 196.2
Liq. Bp_3 107-109°.

Tashiro, M. *et al*, *J.O.C.*, 1978, **43**, 1413 (*synth, ir, pmr*)

3,4-Dimethyldiphenylmethane D-1-00397

1,2-Dimethyl-4-(phenylmethyl)benzene, 9CI. Phenyl-3,4-xylylmethane, 8CI. 4-Benzyl-o-xylene

[13540-56-2]

$C_{15}H_{16}$ M 196.2
Cryst. (EtOH). Mp 27-29°. Bp_{14} 137-138°.

Sisido, K. *et al*, *J.O.C.*, 1961, **26**, 1368 (*synth*)

3,5-Dimethyldiphenylmethane D-1-00398

*1,3-Dimethyl-5-(phenylmethyl)benzene, 9CI. Phenyl-3,5-xylylmethane. 5-Benzyl-*m*-xylene*

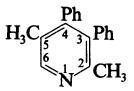
[28122-27-2]

$C_{15}H_{16}$ M 196.2
$Bp_{2.5}$ 121-122°. n_D^{23} 1.5656.

Truce, W.E. *et al*, *J.A.C.S.*, 1958, **80**, 3625 (*synth*)
Mathew, F. *et al*, *Synth. Commun.*, 1995, **25**, 1795 (*pmr, ir*)

2,5-Dimethyl-3,4-diphenylpyridine, 9CI D-1-00399

[79999-04-5]



$C_{19}H_{17}N$ M 259.3
Cryst. Mp 114-115°.

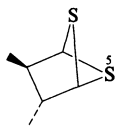
Padwa, A. *et al*, *J.A.C.S.*, 1984, **106**, 1065 (*synth, ir, pmr*)

3,4-Dimethyl-2,6-diphenylpyridine, 9CI D-1-00400

$C_{19}H_{17}N$ M 259.3
Pale brown powder (EtOH). Mp 47-48°.

Jochims, J.C. *et al*, *Synthesis*, 1994, 509 (*synth, cmr, pmr*)

2,3-Dimethyl-5,6-dithiabicyclo[2.1.1]hexane D-1-00401



(2*R**,3*R**)-*form*

$C_6H_{10}S_2$ M 146.2

(2R*,3R*)-form
trans-*form*

5α-Oxide: [120709-22-0]. ***Zwiebelane B***
$C_6H_{10}OS_2$ M 162.2 Constit. of onion (*Allium cepa*). There are four possible isomeric mono-*S*-oxides of the *trans*-form but only this isomer was detected.

(2RS,3SR)-form
cis-*form*

5α-Oxide: [120637-81-2]. ***Zwiebelane A***
$C_6H_{10}OS_2$ M 162.2 Constit. of onion (*A. cepa*). Oil. There are two possible isomeric mono-*S*-oxides of the *cis*-form but only this one was detected.

Bayer, T. *et al*, *J.A.C.S.*, 1989, **111**, 3085; 1990, **112**, 4584 (*isol, struct, synth*)
Block, E. *et al*, *J. Agric. Food Chem.*, 1992, **40**, 2431 (*glc, ms*)

Dimethyldodecylethylammonium(1+) D-1-00402

$H_3C(CH_2)_{11}NMe_2Et^{\oplus}$

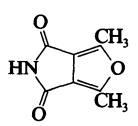
$C_{16}H_{36}N^{\oplus}$ M 242.4 (ion)

Bromide: [68207-00-1].
$C_{16}H_{36}BrN$ M 322.3 Phase transfer catalyst. Mp 185-188°.

Palit, S.R. *et al*, *Trans. Faraday Soc.*, 1959, 463.
Ger. Pat., 2 926 980, (1981); *CA*, **94**, 205041b.

1,3-Dimethyl-4*H*-furo[3,4-*c*]pyrrole-4,6(5*H*)-dione D-1-00403

2,5-Dimethylfuran-3,4-dicarboximide



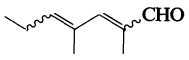
$C_8H_7NO_3$ M 165.1

N-*Me:* [95641-45-5]. *1,3,5-Trimethyl-4H-furo[3,4-c]pyrrole-4,6(5H)-dione, 9CI*
$C_9H_9NO_3$ M 179.1 Needles. Mp 185-186° (sealed tube).

Warrener, R.N. *et al*, *Aust. J. Chem.*, 1995, **48**, 241.

2,4-Dimethyl-2,4-heptadienal, 9CI D-1-00404

[42452-48-2]



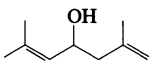
$C_9H_{14}O$ M 138.2
Liq. Bp_{10} 82-83°.

2,4-Dinitrophenylhydrazone: [42452-49-3]. Red needles. Mp 142°.

Seebald, H.J. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1973, **306**, 393 (*synth*)
Hoffmann, R.W. *et al*, *Annalen*, 1994, 837 (*synth, pmr, cmr*)

2,6-Dimethyl-1,5-heptadien-4-ol, 9CI D-1-00405

[19550-64-2]



$C_9H_{16}O$ M 140.2

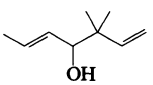
(±)-*form* [124727-43-1]
Liq. Bp_5 69°.

Ac: [77963-75-8].
$C_{11}H_{18}O_2$ M 182.2 Liq. Bp_{17} 68-70°.

Mori, K. *et al*, *Agric. Biol. Chem.*, 1981, **45**, 369 (*synth, Ac, ir, pmr*)
Weyerstahl, P. *et al*, *Annalen*, 1986, 99 (*synth, ir, pmr, cmr, ms*)

3,3-Dimethyl-1,5-heptadien-4-ol, 9CI D-1-00406

[79705-04-7]

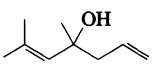


$C_9H_{16}O$ M 140.2
Oil. Bp_{20} 77-79°.

Alder, K. *et al*, *Annalen*, 1957, **609**, 1 (*synth*)
Cohen, T. *et al*, *Synth. Commun.*, 1995, **25**, 33 (*synth, pmr, cmr, ir*)

4,6-Dimethyl-1,5-heptadien-4-ol, 9CI D-1-00407

[926-20-5]



$C_9H_{16}O$ M 140.2

(±)-*form* [123033-25-0]
Liq. Bp 168-170°, Bp_7 55-57°. n_D^{20} 1.4598.

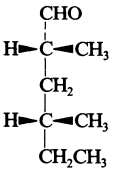
Me ether: 4-Methoxy-4,6-dimethyl-1,5-heptadiene
$C_{10}H_{18}O$ M 154.2 Liq. Bp_{30} 70-71°.

Et ether: 4-Ethoxy-4,6-dimethyl-1,5-heptadiene
$C_{11}H_{20}O$ M 168.2 Liq. Bp_{38} 74-75°.

Henze, H.R. *et al*, *J.O.C.*, 1942, **7**, 326 (*props*)
Sorensen, T.S. *et al*, *Can. J. Chem.*, 1964, **42**, 2781 (*synth*)
Pansevich-Kolyada, V.I. *et al*, *Zh. Obshch. Khim.*, 1965, **1**, 57; *J. Org. Chem. USSR* (*Engl. Transl.*), 1965, **1**, 55 (*ethers, synth*)
Pansevich-Kolyada, V.I. *et al*, *Zh. Obshch. Khim.*, 1970, **40**, 2067; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1970, **40**, 2052 (*synth, ir*)
House, H.O. *et al*, *J.O.C.*, 1978, **43**, 2443 (*synth, ir, pmr*)
Fukuzawa, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1992, **65**, 3308 (*pmr, cmr*)

2,4-Dimethylhexanal D-1-00408

[20514-48-1]



(2*R*,4*R*)-*form*

$C_8H_{16}O$ M 128.2

(2R,4R)-form [62856-65-9]
Pale yellow oil.

2,4-Dinitrophenylhydrazone: Cryst. (EtOH). Mp 112-113°. $[\alpha]_D^{22}$ −37.6 (c, 0.25 in $CHCl_3$).

(±)-*form*

4-Methylbenzenesulfonylhydrazone: Cryst. Mp 62-64°. Mixt. of diastereoisomers.

[42329-87-3, 42330-30-3]

Bertz, S.H. *et al*, *J.O.C.*, 1983, **48**, 116 (*synth, pmr*)
White, J.D. *et al*, *J.O.C.*, 1994, **59**, 3347 (*synth, ir, pmr, cmr, ms*)

3,3-Dimethyl-2,5-hexanedione D-1-00409

$CH_3COC(CH_3)_2CH_2COCH_3$

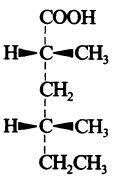
$C_8H_{14}O_2$ M 142.1
Liq. d_{25}^{25} 0.95. Bp_{20} 93°, Bp_{10} 77-78°. n_D^{20} 1.4380.

Bis(semicarbazone): Cryst. (EtOH aq.). Mp 205-206° dec.
Bis(2,4-dinitrophenylhydrazone): Orange-yellow needles (methylcellosolve). Mp 217-218°.

Patrick, T., *J.O.C.*, 1952, **17**, 1269 (*synth*)
Crombie, L. *et al*, *J.C.S.*, 1958, 4417 (*synth, ir*)
Cadman, M.L.F. *et al*, *J.C.S. Perkin 1*, 1995, 1397 (*synth, ir, pmr*)

2,4-Dimethylhexanoic acid D-1-00410

[70621-82-8]



(2*R*,4*R*)-*form*

$C_8H_{16}O_2$ M 144.2

(2R,4R)-form [130248-45-2]
(*2D,4D*)-*form*
Oil. Bp_{20} 125°. $[\alpha]_D^{20}$ −30.6 (c, 3.01 in $CHCl_3$).

(2R,4S)-form [42329-90-8]
(*2D,4L*)-*form*

Me ester:
$C_9H_{18}O_2$ M 158.2 Liq. d_4^{24} 0.87. $[\alpha]_D^{23}$ −8.1.

(2S,4S)-form [42330-37-0]
(2L,4L)-form

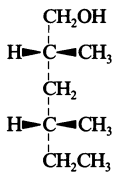
Me ester: Liq. d_4^{22} 0.87. $[\alpha]_D^{24}$ +32.2.

(±)-*form*
Liq. Bp_{18} 113-116°. Prob. mixt. of diastereoisomers.

Stetter, H. *et al, Chem. Ber.*, 1958, **91**, 374 (*synth*)
Frohardt, R.P. *et al, J.A.C.S.*, 1959, **81**, 5500 (*synth*)
Odham, G., *Ark. Kemi*, 1967, **26**, 367 (*synth, gc, ms*)
Bestmann, H.J. *et al, Annalen*, 1988, 55 (*synth, pmr, ir*)
White, J.D. *et al, J.O.C.*, 1994, **59**, 3347 (*synth, ir, pmr, cmr, ms*)

2,4-Dimethyl-1-hexanol D-1-00411

[3965-59-1]



$C_8H_{18}O$ M 130.2
Aroma and taste producing constit. of wine.

(2R,4R)-form [130322-50-8]
Oil. $[\alpha]_D^{22}$ +3.7 (c, 1.67 in $CHCl_3$).

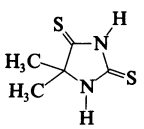
[111675-63-9, 159346-50-6]

Lardicci, L. *et al, Tetrahedron*, 1966, **22**, 1991 (*synth*)
Chenyaga, B.S. *et al, Prikl. Khromatogr.*, 1984, 157; *CA*, **102**, 130376n (*glc*)
White, J.D. *et al, J.O.C.*, 1994, **59**, 3347 (*synth, ir, pmr, cmr, ms*)

5,5-Dimethyl-2,4-imidazolidinedithione, 9CI D-1-00412

5,5-Dimethyl-2,4-dithiohydantoin, 8CI. Thiomedan. Vincidol

[20513-25-1]

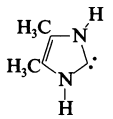


$C_5H_8N_2S_2$ M 160.2
Antiepileptic agent. Pale yellow needles (C_6H_6). Mp 144°.

▶ LD_{50} (mus, ipr) 500 mg/kg. MU0990000.

Carrington, H.C., *J.C.S.*, 1947, 681 (*synth*)
Hazard, R. *et al, C. R. Hebd. Seances Acad. Sci.*, 1948, **226**, 1850; 1949, **228**, 958, 1762; 1950, **230**, 243 (*pharmacol*)
Frommel, E. *et al, Arch. Int. Pharmacodyn. Ther.*, 1952, **92**, 44 (*pharmacol*)
Robbe, Y. *et al, Eur. J. Med. Chem.* (*Chim. Ther.*), 1982, **17**, 235 (*synth, use, tox*)
Cristiani, F. *et al, Spectrochim. Acta A*, 1985, **41**, 487 (*ir*)
Devillanova, F.A. *et al, J. Chem. Res., Synop.*, 1987, **6**, 192 (*cryst struct*)

4,5-Dimethyl-2-imidazolylidene D-1-00413



$C_5H_8N_2$ M 96.1

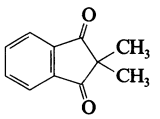
N,N′-*Di-Me: 1,3,4,5-Tetramethyl-2-imidazolylidene*
$C_7H_{12}N_2$ M 124.1 Simple stable carbene. Cryst. (toluene or THF). Mp 109-110°.

Arduengo, A.J. *et al, J.A.C.S.*, 1992, **114**, 5530 (*synth*)

2,2-Dimethyl-1,3-indanedione, 8CI D-1-00414

2,2-Dimethyl-1H-indene-1,3-(2H)-dione, 9CI

[17190-77-1]



$C_{11}H_{10}O_2$ M 174.1
Needles (EtOH aq.). Sol. EtOH, Et_2O, C_6H_6, hot H_2O. Mp 107-108° (101-103.5°).

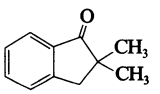
Wislicenus, W. *et al, Annalen*, 1889, **246**, 352 (*synth*)
Nazarov, I.M. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1956, 205; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1956, 197 (*synth*)
Bettembourg, M.-C. *et al, Bull. Soc. Chim. Fr.*, 1963, 2449 (*synth*)
Giovanelli, von K.H. *et al, Ber. Bunsen-Ges. Phys. Chem.*, 1971, **75**, 864 (*uv*)
Watanabe, M. *et al, Synthesis*, 1994, 1083 (*synth, uv, pmr, cmr*)

2,2-Dimethyl-1-indanone D-1-00415

Updated Entry replacing D-0-05812

2,3-Dihydro-2,2-dimethyl-1H-inden-1-one, 9CI

[10489-28-8]



$C_{11}H_{12}O$ M 160.2
Liq.

Orliac-LeMoing, A. *et al, Tetrahedron*, 1985, **41**, 4483 (*synth, ir, pmr*)

2,3-Dimethyl-1-indanone D-1-00416

2,3-Dihydro-2,3-dimethyl-1H-inden-1-one, 9CI

[36230-99-6]

$C_{11}H_{12}O$ M 160.2
Mixt. of *cis*- and *trans*-isomers. Oil. Bp_{10} 118-120°.

[30248-92-1, 30272-59-4]

Barltrop, J.A. *et al, J.C.S.*, 1956, 2928 (*synth*)
Smouno, I. *et al, Synth. Commun.*, 1990, **20**, 1387 (*synth, ir, pmr*)

2,4-Dimethyl-1-indanone D-1-00417

2,3-Dihydro-2,4-dimethyl-1H-inden-1-one, 9CI

[64919-47-7]

$C_{11}H_{12}O$ M 160.2

(±)-*form*
Cryst. Mp 36-37°. Bp_{14} 130-134°.

Bachmann, W.F. *et al, J.C.S.*, 1936, 54 (*synth*)
Elsner, B.B. *et al, J.C.S.*, 1957, 592 (*synth*)

2,5-Dimethyl-1-indanone D-1-00418

2,3-Dihydro-2,5-dimethyl-1H-inden-1-one, 9CI

[89044-48-4]

$C_{11}H_{12}O$ M 160.2

(±)-*form*
Oil. Bp_{14} 136°.

Colonge, J. *et al, Bull. Soc. Chim. Fr.*, 1952, 462 (*synth*)
Fukuoka, M. *et al, Chem. Pharm. Bull.*, 1983, **31**, 3113 (*synth, ir, uv, pmr, cmr*)

2,6-Dimethyl-1-indanone D-1-00419

2,3-Dihydro-2,6-dimethyl-1H-inden-1-one, 9CI

[66309-83-9]

$C_{11}H_{12}O$ M 160.2

(±)-*form*
Oil. Bp_{17} 141-144°.

Colonge, J. *et al, Bull. Soc. Chim. Fr.*, 1951, 961 (*synth*)
Fukuoka, M. *et al, Chem. Pharm. Bull.*, 1983, **31**, 3113 (*synth, ir, uv, pmr, cmr*)

2,7-Dimethyl-1-indanone D-1-00420

2,3-Dihydro-2,7-dimethyl-1H-inden-1-one, 9CI

[89044-49-5]

$C_{11}H_{12}O$ M 160.2

(±)-*form*
Oil. $Bp_{0.04}$ 109°.

Fukuoka, M. *et al, Chem. Pharm. Bull.*, 1983, **31**, 3113 (*synth, ir, uv, pmr, cmr*)

3,3-Dimethyl-1-indanone D-1-00421

2,3-Dihydro-3,3-dimethyl-1H-inden-1-one, 9CI

[26465-81-6]

$C_{11}H_{12}O$ M 160.2
Oil. Bp_{16} 122-125°, $Bp_{0.1}$ 65-71°.

Thompson, H.W. *et al, J.C.S. Perkin 1*, 1976, 1603 (*synth, pmr*)
Quinn, K.J. *et al, Aust. J. Chem.*, 1981, **34**, 685 (*synth, ir, pmr*)
Hillery, P.S. *et al, J.A.C.S.*, 1983, **105**, 2760 (*synth, ir, pmr*)

3,4-Dimethyl-1-indanone D-1-00422

2,3-Dihydro-3,4-dimethyl-1H-inden-1-one, 9CI

[35322-82-8]

$C_{11}H_{12}O$ M 160.2

(±)-*form*
Oil.

Kemp, W. *et al, J.C.S. Perkin 1*, 1972, 151 (*synth, ir, pmr*)
Vickery, E.H. *et al, Org. Prep. Proced. Int.*, 1979, **11**, 255 (*synth*)

3,6-Dimethyl-1-indanone D-1-00423

2,3-Dihydro-3,6-dimethyl-1H-inden-1-one, 9CI

[17714-94-2]

$C_{11}H_{12}O$ M 160.2

(±)-*form*
Oil. Bp_{10} 130-134°, Bp_5 100-102°.

Pines, H. *et al*, *J.A.C.S.*, 1949, **71**, 3534 (*synth*)
Elsner, B.B. *et al*, *J.C.S.*, 1957, 592 (*synth*)
Kemp, W. *et al*, *J.C.S. Perkin 1*, 1972, 151 (*synth*, *pmr*)

3,7-Dimethyl-1-indanone D-1-00424

2,3-Dihydro-3,7-dimethyl-1H-inden-1-one, *9CI*

$C_{11}H_{12}O$ M 160.2

(±)-*form*
Oil. $Bp_{0.3}$ 75-77°.

[40267-38-7]

Tada, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 549 (*synth*, *ir*, *uv*)
Allen, J.M. *et al*, *Tetrahedron*, 1977, **33**, 2083 (*synth*)

4,5-Dimethyl-1-indanone D-1-00425

2,3-Dihydro-4,5-dimethyl-1H-inden-1-one, *9CI*

[37678-61-8]

$C_{11}H_{12}O$ M 160.2
Needles. Mp 99°.

Hart, R.T. *et al*, *J.A.C.S.*, 1950, **72**, 3286 (*synth*)
Nakada, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 2243 (*ir*, *uv*, *pmr*)
Bartmann, W. *et al*, *J. Het. Chem.*, 1987, **24**, 677 (*synth*)

4,6-Dimethyl-1-indanone D-1-00426

2,3-Dihydro-4,6-dimethyl-1H-inden-1-one

[1685-81-0]

$C_{11}H_{12}O$ M 160.2
Cryst. Mp 121°.

Bartmann, W. *et al*, *J. Het. Chem.*, 1987, **24**, 677 (*synth*)

4,7-Dimethyl-1-indanone D-1-00427

2,3-Dihydro-4,7-dimethyl-1H-inden-1-one

[5037-60-5]

$C_{11}H_{12}O$ M 160.2
Cryst. Mp 78-79°.

Bartmann, W. *et al*, *J. Het. Chem.*, 1987, **24**, 677 (*synth*)
Frim, R. *et al*, *Chem. Ber.*, 1989, **122**, 737 (*synth*, *ir*, *pmr*, *ms*)

5,6-Dimethyl-1-indanone D-1-00428

2,3-Dihydro-5,6-dimethyl-1H-inden-1-one, *9CI*

[16440-97-4]

$C_{11}H_{12}O$ M 160.2
Cryst. (petrol). Mp 87-88°.

Sliwa, H., *Bull. Soc. Chim. Fr.*, 1970, 631 (*synth*, *ir*, *pmr*)
Bartmann, W. *et al*, *J. Het. Chem.*, 1987, **24**, 677 (*synth*)

5,7-Dimethyl-1-indanone D-1-00429

2,3-Dihydro-5,7-dimethyl-1H-inden-1-one, *9CI*

[6682-69-5]

$C_{11}H_{12}O$ M 160.2
Needles. Mp 76-77°.

Bergmark, W.R. *et al*, *J.O.C.*, 1985, **50**, 5612 (*ir*, *pmr*)
Bartmann, W. *et al*, *J. Het. Chem.*, 1987, **24**, 677 (*synth*)

6,7-Dimethyl-1-indanone D-1-00430

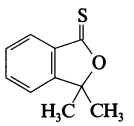
2,3-Dihydro-6,7-dimethyl-1H-inden-1-one, *9CI*

[16440-98-5]

$C_{11}H_{12}O$ M 160.2
Cryst. Mp 47-50°.

Bartmann, W. *et al*, *J. Het. Chem.*, 1987, **24**, 677 (*synth*)

3,3-Dimethyl-1(3*H*)-isobenzofuranthione D-1-00431



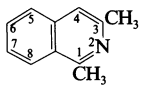
$C_{10}H_{10}OS$ M 178.2
Cryst. Mp 33-34°. Bp_3 130°.

Nishio, T., *J.C.S. Perkin 1*, 1995, 561 (*synth*, *ir*, *pmr*, *cmr*)

1,3-Dimethylisoquinoline, 9CI D-1-00432

Updated Entry replacing D-0-09761

[1721-94-4]



$C_{11}H_{11}N$ M 157.2
Bp_{15} 134-135°.
Picrate: [73480-90-7]. Mp 181-182°.

Fitton, A.O. *et al*, *Chem. Comm.*, 1973, 889 (*synth*)
Zielinski, W., *Synthesis*, 1980, 70 (*synth*, *spectra*)
Mukkala, V. *et al*, *Helv. Chim. Acta*, 1992, **75**, 1621 (*synth*, *uv*, *pmr*)

1,4-Dimethylisoquinoline, 9CI D-1-00433

[1721-95-5]

$C_{11}H_{11}N$ M 157.2
Oil. $Bp_{0.05}$ 78-82°.
Picrate: Cryst. Mp 225°.
N-*Oxide:* [35967-07-8]. $C_{11}H_{11}NO$ M 173.2 Cryst. Mp 50-51°.

Späth, F. *et al*, *Ber., B*, 1930, **63**, 134 (*synth*)
Krabbe, W. *et al*, *Ber., B*, 1941, **74**, 1905 (*synth*)
Agrawal, K.C. *et al*, *J. Med. Chem.*, 1972, **15**, 192; 1976, **19**, 970 (*synth*, *pmr*)

1,5-Dimethylisoquinoline D-1-00434

[72678-15-0]

$C_{11}H_{11}N$ M 157.2
Picrate: Cryst. Mp 230-231°.

Spath, F. *et al*, *Ber., B*, 1930, **63**, 134 (*synth*)

1,6-Dimethylisoquinoline, 9CI D-1-00435

$C_{11}H_{11}N$ M 157.2
Bp_{20} 160-165°.
Picrate: Yellow needles (EtOH). Mp 225-227°.

Quelet, R. *et al*, *C. R. Hebd. Seances Acad. Sci.*, 1957, **244**, 909 (*synth*)
Vinot, N., *Ann. Chim. (Paris)*, 1958, **3**, 461 (*synth*)
Jones, G., *J.C.S.*, 1960, 1918 (*synth*, *uv*)

1,7-Dimethylisoquinoline D-1-00436

$C_{11}H_{11}N$ M 157.2
Mp 35-37°. Bp_{15} 148-150°.
Picrate: Yellow prisms (EtOH). Mp 223-224°.

Jones, G., *J.C.S.*, 1960, 1918 (*synth*, *uv*)

1,8-Dimethylisoquinoline, 9CI D-1-00437

[102878-54-6]

$C_{11}H_{11}N$ M 157.2
Mp 49-51°.

Jones, G., *J.C.S.*, 1960, 1918 (*synth*)

3,4-Dimethylisoquinoline, 9CI D-1-00438

$C_{11}H_{11}N$ M 157.2
Picrate: Cryst. (H_2O). Mp 224-226° (212-213°).

[37978-64-6]

Witkop, B., *J.A.C.S.*, 1948, **70**, 1424 (*synth*)
Jones, G., *J.C.S.*, 1960, 1896 (*synth*)

3,5-Dimethylisoquinoline D-1-00439

$C_{11}H_{11}N$ M 157.2
Picrate: Pale yellow needles (EtOH). Mp 219-220°.

Gibson, M.S., *J.C.S.*, 1956, 808 (*synth*)

3,6-Dimethylisoquinoline, 9CI D-1-00440

[102878-58-0]

$C_{11}H_{11}N$ M 157.2
Cryst. Mp 78-79°.
Picrate: Cryst. Mp 209-211° (193-195°).

Vinot, N., *Bull. Soc. Chim. Fr.*, 1960, 617 (*synth*)
Kido, K. *et al*, *Chem. Pharm. Bull.*, 1987, **35**, 4964 (*synth*, *uv*)

4,5-Dimethylisoquinoline D-1-00441

$C_{11}H_{11}N$ M 157.2
Picrate: Yellow needles (Me_2CO). Mp 234-235°.

Gibson, M.S., *J.C.S.*, 1956, 808 (*synth*)

4,7-Dimethylisoquinoline D-1-00442

$C_{11}H_{11}N$ M 157.2
Bp_{15} 140°.
Picrate: Yellow prisms (EtOH). Mp 223°.

Jones, G., *J.C.S.*, 1960, 1918 (*synth*, *uv*)

5,7-Dimethylisoquinoline, 9CI D-1-00443

[72374-17-5]

$C_{11}H_{11}N$ M 157.2
Picrate: Yellow needles (EtOH). Mp 261-262° dec.

Gibson, M.S., *J.C.S.*, 1956, 808 (*synth*)
Gilchrist, T.L. *et al*, *Chem. Comm.*, 1979, 627 (*synth*)

5,8-Dimethylisoquinoline, 9CI D-1-00444

[75476-82-3]

$C_{11}H_{11}N$ M 157.2
Picrate: Yellow needles (EtOH). Mp 233-236°.
N-*Oxide:* [155826-17-8]. $C_{11}H_{11}NO$ M 173.2 Needles (EtOH). Mp 146-149°.

Miller, R.B. *et al*, *J.O.C.*, 1980, **45**, 5312 (*synth*)
Marsais, F. *et al*, *J. Het. Chem.*, 1988, **25**, 81 (*synth, pmr*)
Boogaard, A.J. *et al*, *Tetrahedron*, 1994, **50**, 4811 (*synth, ir, pmr, ms*)

6,8-Dimethylisoquinoline, 9CI D-1-00445

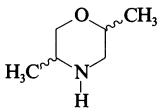
[67878-83-5]

$C_{11}H_{11}N$ M 157.2

Su, J.-A. *et al*, *Org. Magn. Reson.*, 1977, **10**, 122 (*synth, cmr*)

2,5-Dimethylmorpholine, 9CI D-1-00446

[106-56-9]

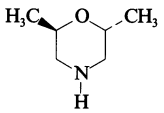


$C_6H_{13}NO$ M 115.1
Liq. Bp 145°. n_D^{16} 1.4459.

Berlin, A.Ya. *et al*, *Zh. Obshch. Khim.*, 1950, **20**, 640; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1950, **20**, 677 (*synth*)
Hernestam, S. *et al*, *Org. Magn. Reson.*, 1978, **11**, 116 (*cmr*)

2,6-Dimethylmorpholine, 9CI D-1-00447

[141-91-3]



(*2RS,6RS*)-*form*

$C_6H_{13}NO$ M 115.1

(***2RS,6RS*)-*form*** [6485-45-6]
(±)-trans-*form*
Liq. $n_D^{22.3}$ 1.4480.

Picrate: Yellow needles. Mp 161-162°.

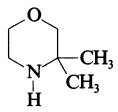
(***2RS,6SR*)-*form*** [6485-55-8]
cis-*form*
Liq. Bp 142°. $n_D^{22.3}$ 1.4438.

Picrate: Yellow needles (EtOH). Mp 199-200°.

U.K. Pat., 298 336, (1927); *CA*, **23**, 2723 (*synth*)
Booth, H. *et al*, *Tetrahedron*, 1965, **21**, 3429 (*purif, pmr*)
Hernestam, S. *et al*, *Org. Magn. Reson.*, 1978, **11**, 116 (*cmr*)

3,3-Dimethylmorpholine, 9CI D-1-00448

[59229-63-9]

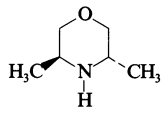


$C_6H_{13}NO$ M 115.1
Liq. Bp 143-144°. n_D^{20} 1.4472.

Cottle, D.L. *et al*, *J.O.C.*, 1946, **11**, 286 (*synth*)
Jones, A.J. *et al*, *Can. J. Chem.*, 1976, **54**, 126 (*cmr*)

3,5-Dimethylmorpholine, 9CI D-1-00449

[123-57-9]



(3*S*,5*S*)-*form*

$C_6H_{13}NO$ M 115.1

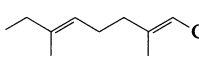
(***3S,5S*)-*form*** [154634-96-5]
(+)-trans-*form*
Oil. Bp_{65} 75°. $[\alpha]_D^{20}$ +38.3 (neat).

Berlin, A.Ya. *et al*, *Zh. Obshch. Khim.*, 1950, **20**, 640; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1950, **20**, 677 (*synth*)
Hernestam, S. *et al*, *Org. Magn. Reson.*, 1978, **11**, 116 (*cmr*)
Enders, D. *et al*, *Synthesis*, 1994, 66 (*synth, pmr, cmr*)

3,7-Dimethyl-2,6-nonadienal, 9CI D-1-00450

Ethyl citral

[41448-29-7]



(*E,E*)-*form*

$C_{11}H_{18}O$ M 166.2
Used in perfumery and in synth. of juvenile hormone analogues. Yellow liq. with strong lemon scent. d 0.89.

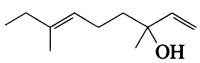
[70173-14-7, 70173-15-8, 121952-89-4]

Freeman, R.K. *et al*, *Tetrahedron*, 1988, **44**, 5051 (*synth, pmr, ir, ms*)

3,7-Dimethyl-1,6-nonadien-3-ol D-1-00451

Ethyllinalool

[10339-55-6]



$C_{11}H_{20}O$ M 168.2
Used in perfumery. d 0.86. Bp 45-50°. n_D^{30} 1.4580.

Ac: [61931-80-4]. *Ethyllinalyl acetate* $C_{13}H_{22}O_2$ M 210.3 Used in perfumery. d 0.90. n_D^{20} 1.45.

[54592-32-4, 92590-71-1]

Mori, K. *et al*, *Tetrahedron*, 1969, **25**, 1667.
Krimer, M.Z. *et al*, *Zh. Org. Khim.*, 1974, **10**, 1614.
Vaidya, N.A. *et al*, *Indian J. Chem., Sect. B*, 1984, **23**, 241.

2,2-Dimethylpentanoic acid, 9CI D-1-00452

2,2-Dimethylvaleric acid, 8CI

[1185-39-3]

$H_3CCH_2CH_2C(CH_3)_2COOH$

$C_7H_{14}O_2$ M 130.1
Liq. d_4^{20} 0.9189. Bp_9 98-99°. n_D^{20} 1.4212.

Me ester: [813-68-3].
$C_8H_{16}O_2$ M 144.2 Liq. Bp 144-145°.

Et ester: [5837-93-4].
$C_9H_{18}O_2$ M 158.2 Liq. Bp 161.0-161.5°.

Chloride: [15721-22-9].
$C_7H_{13}ClO$ M 148.6 Liq. Bp_{10} 45°.

Amide: [13146-36-6].
$C_7H_{15}NO$ M 129.2 Mp 95-96°.

Nitrile: [20654-47-1]. *2-Cyano-2-methylpentane*
$C_7H_{13}N$ M 111.1 Liq. Bp_{40} 60°.

Locquin, R. *et al*, *Bull. Soc. Chim. Fr.*, 1926, **39**, 433 (*Me ester, chloride, amide*)
Terent'ev, A.B. *et al*, *Org. Magn. Reson.*, 1977, **9**, 301 (*cmr*)
Rüchardt, C. *et al*, *Chem. Ber.*, 1981, **114**, 3831; 1994, **127**, 2225 (*nitrile, synth*)

3,3-Dimethyl-1-penten-4-yne, 9CI D-1-00453

[43219-81-4]

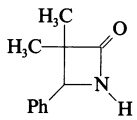
$HC{\equiv}CC(CH_3)_2CH{=}CH_2$

C_7H_{10} M 94.1
Liq. d_4^{20} 0.72. Bp 67-68°. n_D^{20} 1.4050.

Peiffer, G., *C. R. Hebd. Seances Acad. Sci.*, 1964, **258**, 3499 (*synth*)
Bubnov, Y.N. *et al*, *Synthesis*, 1980, 904 (*synth, pmr*)
Barbot, F. *et al*, *J. Organomet. Chem.*, 1992, **440**, 249 (*synth, ir, pmr*)
Roth, W.R. *et al*, *Annalen*, 1995, 1061 (*synth, pmr, ir, ms*)

3,3-Dimethyl-4-phenyl-2-azetidinone D-1-00454

[7486-93-3]



$C_{11}H_{13}NO$ M 175.2

(±)-*form*
Mp 104-105°.

Colvin, E.W. *et al*, *Tetrahedron*, 1988, **44**, 4157.
Ishihara, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1995, **68**, 1721 (*synth*)

3,3-Dimethyl-1-phenyl-2-butylamine D-1-00455

α-(*1,1-Dimethylethyl*)*benzeneethanamine, 9CI. 2-Amino-3,3-dimethyl-1-phenylbutane*

[67309-37-9]

$(H_3C)_3CCH(NH_2)CH_2Ph$

$C_{12}H_{19}N$ M 177.2

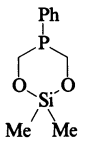
(±)-***form*** [84524-60-7]
Oil.

Hydrochloride: [84524-43-6].
Mp 189-190°.

Hall, S.S. *et al*, *J.O.C.*, 1986, **51**, 5338 (*synth, ir, pmr, ms*)
Katritzky, A.R. *et al*, *Synth. Commun.*, 1994, **24**, 2955 (*synth*)

2,2-Dimethyl-5-phenyl-1,3-dioxa-5-phospha-2-silacyclohexane, 9CI D-1-00456

[71787-50-3]



$C_{10}H_{15}O_2PSi$ M 226.2
Synth. from $PhP(CH_2OH)_2$ + Me_2SiCl_2. Liq. Bp_3 95-97°. n_D^{18} 1.5392.

5-Sulfide: [80202-58-0].
$C_{10}H_{15}O_2PSSi$ M 258.3 Solid. Mp 80-81°.

5-Selenide: [93594-04-8].
$C_{10}H_{15}O_2PSeSi$ M 305.2 Liq. $Bp_{0.03}$ 148-151°.

[83264-13-5]

Voronkov, M.G. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1979, **247**, 609; *Dokl. Chem. (Engl. Transl.)*, 1979, **247**, 355 (*synth, ir, P-31 nmr, conformn*)
Gluklikh, V.I. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1979, **247**, 1179; *Dokl. Phys. Chem. (Engl. Transl.)*, 1979, **247**, 682 (*pmr, cmr, P-31 nmr*)
Voronkov, M.G. *et al, Zh. Obshch. Khim.*, 1981, **51**, 2176; *J. Gen. Chem. USSR (Engl. Transl.)*, 1981, **51**, 1872 (*sulfide, ms, P-31 nmr*)
Panov, A.M. *et al, Zh. Obshch. Khim.*, 1981, **51**, 2631; *J. Gen. Chem. USSR (Engl. Transl.)*, 1981, **51**, 2269 (*sulfide, synth, ms, P-31 nmr*)
Kirillova, N.I. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1984, **278**, 366 (*cryst struct*)
Patsanovskii, I.I. *et al, Zh. Obshch. Khim.*, 1984, **54**, 1738; *J. Gen. Chem. USSR (Engl. Transl.)*, 1984, **54**, 1549 (*sulfide, selenide, pmr, cmr, P-31 nmr, Se-77 nmr*)
Zyablikova, T.A. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1990, 776; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1990, 688 (*selenide, P-31 nmr, Se-77 nmr*)

(2,3-Dimethylphenyl) hydrazine, 9CI D-1-00457

2,3-Xylylhydrazine

[84401-19-4]

$C_8H_{12}N_2$ M 136.1
Needles (AcOH). Mp 108°.

Monohydrochloride: [56737-75-8].
Plates (AcOH). Mp 208°.

Franzen, H. *et al, J. Prakt. Chem.*, 1918, **97**, 344 (*synth*)
Marion, L. *et al, Can. J. Res., Sect. B*, 1947, **25**, 1 (*synth*)

(2,4-Dimethylphenyl) hydrazine, 9CI D-1-00458

2,4-Xylylhydrazine

[615-00-9]

$C_8H_{12}N_2$ M 136.1
Cryst. Mp 85°.

Monohydrochloride: [60480-83-3].
Cryst. Mp 184-186°.
Monopicrate: [24006-16-4].
Yellow cryst. (EtOH). Mp 135-136° dec.
Hunsberger, I.M. *et al, J.O.C.*, 1956, **21**, 394 (*synth*)
Kauffmann, T. *et al, Chem. Ber.*, 1969, **102**, 3088 (*synth*)

(2,5-Dimethylphenyl) hydrazine, 9CI D-1-00459

2,5-Xylylhydrazine

[613-85-4]

$C_8H_{12}N_2$ M 136.1
Cryst. Mp 78°.

Monohydrochloride: [56737-78-1].
Cryst. Mp 209°.
Monopicrate: [24006-17-5].
Yellow needles. Mp 133-134°.

[73058-75-0]

Carlin, R.B. *et al, J.A.C.S.*, 1959, **81**, 4673 (*synth*)
Kauffmann, T. *et al, Chem. Ber.*, 1969, **102**, 3088 (*synth*)

(2,6-Dimethylphenyl) hydrazine, 9CI D-1-00460

2,6-Xylylhydrazine

[603-77-0]

$C_8H_{12}N_2$ M 136.1
Long needles (petrol). Mp 36-40°.

Monohydrochloride: [2538-61-6].
Needles (EtOH). Mp 211° dec.

[78157-43-4]

Carlin, R.B. *et al, J.A.C.S.*, 1959, **81**, 4673 (*synth*)

(3,4-Dimethylphenyl) hydrazine, 9CI D-1-00461

3,4-Xylylhydrazine

[13636-53-8]

$C_8H_{12}N_2$ M 136.1
Yellow needles (Et_2O). Mp 57°.

Monohydrochloride: [60481-51-8].
Cryst. (H_2O). Mp 197° dec.
Monopicrate: [24006-18-6].
Yellow needles. Mp 142-143°.

[86746-50-1]

Franzen, H. *et al, J. Prakt. Chem.*, 1918, **97**, 344 (*synth*)
Kauffmann, T. *et al, Chem. Ber.*, 1969, **102**, 3088 (*synth*)

(3,5-Dimethylphenyl) hydrazine, 9CI D-1-00462

3,5-Xylylhydrazine

[39943-61-8]

$C_8H_{12}N_2$ M 136.1
Cryst. Mp 80-82°. Sensitive to air and light.

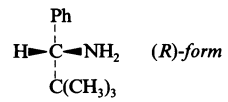
[60481-36-9]

Borsche, W. *et al, Annalen*, 1941, **549**, 238 (*synth*)
Snyder, H.R. *et al, J.A.C.S.*, 1953, **75**, 1873 (*synth*)

2,2-Dimethyl-1-phenyl-1-propylamine D-1-00463

α-(1,1-Dimethylethyl)benzenemethanamine, 9CI. α-tert-Butylbenzylamine, 8CI

[61501-04-0]



(R)-form

$C_{11}H_{17}N$ M 163.2

(R)-form [3082-71-1]
Oil. Bp_{14} 99-101°. $[\alpha]_D^{21}$ +5.6 (neat), $[\alpha]_D^{21}$ +2.5 (c, 4 in MeOH).
Hydrochloride: [19068-35-0].
Cryst. (EtOH/Et_2O). $[\alpha]_D^{26}$ +5.5 (c, 2 in EtOH). Sublimes at 200°.
N-*Ac:* [2975-91-9].
$C_{13}H_{19}NO$ M 205.2 Solid. Mp 135-137°. $Subl._{0.02}$ 100°. $[\alpha]_D^{28}$ +77.0 (c, 2.01 in EtOH).

(S)-form [82729-98-4]
Oil. Bp_{28} 115-117°, $Bp_{0.25}$ 45°. $[\alpha]_D^{25}$ −5.4 (neat), $[\alpha]_D^{24}$ −2.26 (c, 5.3 in MeOH) (90% ee).
Hydrochloride: [108082-57-1].
$[\alpha]_D^{25}$ −5.0 (c, 1.6 in EtOH).

(±)-form [42070-95-1]
Oil. Bp_{22} 115°.
Hydrochloride: Cryst. (EtOH). Mp 220° dec.
N-*Formyl:* [42071-02-3].
$C_{12}H_{17}NO$ M 191.2 Cryst. (petrol). Mp 66-67°.
N-*Ac:* Cubes (EtOH aq.). Mp 133-134°.
N-*Me:* [42071-11-4].
$C_{12}H_{19}N$ M 177.2 Liq. Bp_{10} 92-92.5°.

Billon, P., *Ann. Chim. (Paris)*, 1927, **7**, 314 (*synth*)
Smith, H.E. *et al, J.A.C.S.*, 1965, **87**, 1757; 1987, **109**, 3361 (*synth, resoln, uv*)
Smith, H.E. *et al, J.O.C.*, 1965, **30**, 2654 (*Ac, synth*)
Červinka, O. *et al, Coll. Czech. Chem. Comm.*, 1970, **35**, 721; 1973, **38**, 441 (*synth, Ac, formyl*)
Hall, S.S. *et al, J.O.C.*, 1986, **51**, 5338 (*synth, ir, pmr, ms*)
Dieter, R.K. *et al, Can. J. Chem.*, 1994, **71**, 814 (*synth, pmr, cmr*)

N,N'-Dimethyl-*N*-phenylurea, 9CI D-1-00464

Vulpex

[938-91-0]

MeNHCONMePh

$C_9H_{12}N_2O$ M 164.2
Shows herbicidal props. Cryst. (EtOH). Mp 78-81°.

Briody, T.A. *et al, Tetrahedron*, 1977, **33**, 1469 (*synth*)

P-[2-(Dimethylphosphino) ethyl]-*N,N,N',N'*-tetramethylphosphonous diamide D-1-00465

[*2-(Dimethylphosphino)ethyl*]*phosphonous bis(dimethylamide)*

[63578-30-3]

$Me_2PCH_2CH_2P(NMe_2)_2$

$C_8H_{22}N_2P_2$ M 208.2

Ligand. Liq. $Bp_{0.007}$ 40-45°.

King, R.B. *et al*, *J.A.C.S.*, 1977, **99**, 4001 (*synth, pmr, cmr, P-31 nmr*)

Dimethylphosphinylacetic acid D-1-00466

[6226-01-3]

$Me_2P(O)CH_2COOH$

$C_4H_9O_3P$ M 136.0

Oil which cryst. (MeCN/EtOAc). Mp 97-98°, Mp 105-106°. Hygroscopic.

Et ester: [17534-98-4]. *Ethyl dimethylphosphinyl acetate* $C_6H_{13}O_3P$ M 164.1 Cryst. (Et_2O/hexane). Mp 42.5-43.5°. Bp_1 147-149°.

Gladshtein, B.M. *et al*, *Zh. Obshch. Khim.*, 1967, **37**, 2055; *J. Gen. Chem. USSR (Engl. Transl.)*, 1967, **37**, 1949 (*ester*)

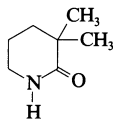
Malevannaya, R. *et al*, *Zh. Obshch. Khim.*, 1971, **41**, 2359; *J. Gen. Chem. USSR (Engl. Transl.)*, 1971, **41**, 2385 (*ester*)

Tsvetkov, E.N. *et al*, *Zh. Obshch. Khim.*, 1974, **44**, 1225; *J. Gen. Chem. USSR (Engl. Transl.)*, 1974, **44**, 1203 (*pmr, props*)

Chen, J. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **63**, 403 (*synth, pmr, cmr, P-31 nmr*)

3,3-Dimethyl-2-piperidinone, 9CI D-1-00467

[23789-83-5]



$C_7H_{13}NO$ M 127.1

Solid (CH_2Cl_2/hexane). Mp 106-108° (102-103°).

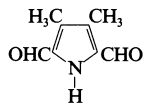
Fr. Pat., 1 527 755, (1968); *CA*, **71**, 91328t (*synth*)

Padwa, A. *et al*, *Synthesis*, 1994, 993 (*synth, ir, pmr, cmr*)

3,4-Dimethyl-1*H*-pyrrole-2,5-dicarboxaldehyde, 9CI D-1-00468

*2,5-Diformyl-3,4-dimethyl-1*H*-pyrrole*

[51952-99-9]



$C_8H_9NO_2$ M 151.1

Cryst. (CH_2Cl_2/hexane). Mp 155-158.5°.

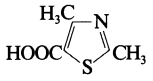
Fischer, H. *et al*, *Annalen*, 1938, **533**, 216 (*synth*)

Battersby, A.R. *et al*, *J.C.S. Perkin 1*, 1984, 2733 (*synth, pmr*)

Cadamuro, S. *et al*, *J.C.S. Perkin 1*, 1993, 2939 (*synth, ir*)

2,4-Dimethyl-5-thiazolecarboxylic acid D-1-00469

[53137-27-2]



$C_6H_7NO_2S$ M 157.1

Anilide: [21452-18-6]. ***Metsulfovax, BSI, ANSI.*** *2,4-Dimethyl-*N*-phenyl-5-thiazolecarboxamide, 9CI. 2,4-Dimethyl-1,3-thiazole-5-carboxanilide. Provax* $C_{12}H_{12}N_2OS$ M 232.3 Systemic fungicide. Cryst. Mp 140-142°. pK_a 2.05.

▶ LD_{50} (rat, orl) 3929 mg/kg.

[35019-85-3]

Mathre, D.E., *J. Agric. Food Chem.*, 1971, **19**, 872 (*activity*)

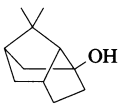
Abdel-Lateef, M.F.A. *et al*, *Acta Phytopathol. Acad. Sci. Hung.*, 1973, **8**, 269, 283 (*synth, activity*)

White, G.A., *Pestic. Biochem. Physiol.*, 1989, **34**, 255 (*synth, fungic activity*)

Pesticide Manual, 9th edn., 1991, No. 8582.

8,8-Dimethyltricyclo[4.2.1.$0^{3,7}$]nonan-6-ol D-1-00470

Fortesol



$C_{11}H_{18}O$ M 166.2

Revised struct. based on cryst. struct. detn. Semisynthetic monoterpenoid obt. by rearr. of (Nopol). Cryst. (petrol or Et_2O). Mp 75-77° (60-63°).

Giddings, R.M. *et al*, *J.C.S. Perkin 2*, 1986, 1525 (*synth, ir, cmr*)

Fortes, A.G. *et al*, *Acta Cryst. C*, 1995, **51**, 914 (*cryst struct*)

1,1-Dimethyl-2-(trifluoromethyl)diphosphine, 9CI D-1-00471

[117583-73-0]

$Me_2P—PHCF_3$

$C_3H_7F_3P_2$ M 162.0

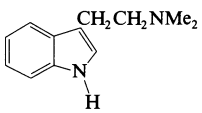
Liq. at −78°. Sol. org. solvs. V.p. 19 mm at 25°. Stable for 1 week at ambient temp.

Avens, L.R. *et al*, *Inorg. Chem.*, 1989, **28**, 200, 205 (*synth, ir, F-19 nmr, P-31 nmr*)

N,N-Dimethyltryptamine D-1-00472

N,N-*Dimethyl-1*H*-indole-3-ethanamine, 9CI. **Nigerine.** DMT*

[61-50-7]



$C_{12}H_{16}N_2$ M 188.2

Alkaloid from *Mimosa hostilis*, *Acacia* spp., *Arundo donax*, *Desmodium* spp., *Phalaris* spp., *Banisteriopsis argentea*, *Psychotria* spp., *Virola peruviana*, *Zanthoxylum* spp. and others (Leguminosae, Gramineae, Malphigiaceae, Rubiaceae, Myristicaceae, Rutaceae). Shows affinity for $5HT_{1D}$-receptor sites. Shows hallucinogenic props. Drug of abuse. Mp 48-49° (39-44°).

▶ LD_{50} (mus, ipr) 47 mg/kg. NL7350000.

Methiodide: Mp 215-216°.

Picrate: Yellow (stable) or red (metastable) cryst. Mp 171-172°.

N^b-*Oxide:* [948-19-6]. **N,N-*Dimethyltryptamine* N-oxide** $C_{12}H_{16}N_2O$ M 204.2 Alkaloid from *Desmodium pulchellum*, *D. triflorum* and other *D.* spp., also *Piptadenia peregrina* and *P. pulchellum* (Leguminosae). Hydrate. Mp 123-128°.

N^b-*Oxide, picrate:* Cryst. (EtOH). Mp 178-183°.

Fish, M.S. *et al*, *J.A.C.S.*, 1955, **77**, 5892 (*isol, oxide*)

Hochstein, F.A. *et al*, *J.A.C.S.*, 1957, **79**, 5735 (*isol*)

Pachter, I.J. *et al*, *J.O.C.*, 1959, **24**, 1285 (*isol*)

Culvenor, C.C.J. *et al*, *Aust. J. Chem.*, 1964, **17**, 1301 (*isol*)

Fitzgerald, J.S. *et al*, *Aust. J. Chem.*, 1965, **18**, 433 (*isol*)

Ghosal, S. *et al*, *J.O.C.*, 1966, **31**, 2284 (*isol*)

Falkenberg, G., *Acta Cryst. B*, 1972, **28**, 3075 (*cryst struct*)

Couch, M.W. *et al*, *Anal. Biochem.*, 1972, **50**, 612 (*ms*)

Grina, J.A. *et al*, *J.O.C.*, 1982, **47**, 2648 (*isol, uv, pmr, cmr*)

Sitaram, B.R. *et al*, *Biochem. Pharmacol.*, 1987, **36**, 1509 (*metab*)

Glennon, R.A. *et al*, *Drug Dev. Res.*, 1991, **22**, 25 (*sar*)

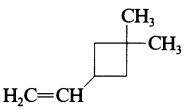
Strassman, R.J. *et al*, *Arch. Gen. Psychiatry*, 1994, **51**, 85, 98 (*pharmacol, human*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DPF600.

1,1-Dimethyl-3-vinylcyclobutane D-1-00473

3-Ethenyl-1,1-dimethylcyclobutane, 9CI

[52708-22-2]



C_8H_{14} M 110.1

Liq. Bp 82°.

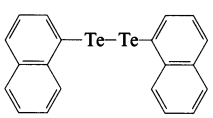
Bruckmann, P. *et al*, *Chem. Ber.*, 1974, **107**, 1108; 1978, **111**, 944 (*synth, ir, pmr*)

Ashby, E.C. *et al*, *Acta Chem. Scand.*, 1990, **44**, 291.

Ashby, E.C. *et al*, *J.O.C.*, 1993, **58**, 424 (*synth, pmr, ms*)

Di-1-naphthalenyl ditelluride D-1-00474

[32294-58-9]



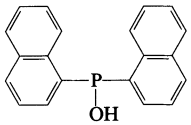
$C_{20}H_{14}Te_2$ M 509.5

Brown solid. Mp 112°.

Crich, D. *et al*, *J.A.C.S.*, 1994, **116**, 8937 (*synth, pmr*)

Di-1-naphthalenylphosphonous acid D-1-00475

Di-1-naphthylphosphinous acid



$C_{20}H_{15}OP$ M 302.3

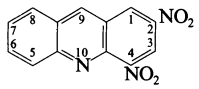
Chloride: [36042-99-6].
$C_{20}H_{14}ClP$ M 320.7 Solid. Mp 130-132°. $Bp_{0.6}$ 227-229°, Bp_{15} 270-280°.

Bromide: [32186-91-7].
$C_{20}H_{14}BrP$ M 365.2 Solid. Mp 29-30°. $Bp_{0.15}$ 280-300°.

Weinberg, K.G., *J.O.C.*, 1975, **40**, 3586.

2,4-Dinitroacridine D-1-00476

Updated Entry replacing D-0-11069
1,3-Dinitroacridine (obsol.)
[79110-36-4]



$C_{13}H_7N_3O_4$ M 269.2
Brownish-orange needles (Py). Mp 284°.

Mayer, F. *et al*, *Ber.*, 1917, **50**, 1314 (*synth*)
Albert, A. *et al*, *J.C.S.*, 1938, 25 (*synth*)
Rosevear, J. *et al*, *Aust. J. Chem.*, 1981, **34**, 839 (*synth, pmr*)

2,6-Dinitroacridine, 9CI D-1-00477

[79110-23-9]
$C_{13}H_7N_3O_4$ M 269.2
Cryst. (AcOH). Mp 272-274°.

Rosevear, J. *et al*, *Aust. J. Chem.*, 1981, **34**, 839 (*synth, pmr*)

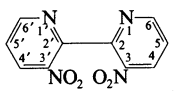
2,7-Dinitroacridine, 9CI D-1-00478

[79110-24-0]
$C_{13}H_7N_3O_4$ M 269.2
Cryst. (AcOH). Mp 322-324°.

Rosevear, J. *et al*, *Aust. J. Chem.*, 1981, **34**, 839 (*synth, pmr*)

3,3′-Dinitro-2,2′-bipyridine, D-1-00479

9CI
[1024-94-8]



$C_{10}H_6N_4O_4$ M 246.1
Cryst. (dioxan). Mp 210-211°.

Kanoktanaporn, S. *et al*, *J.C.S. Perkin 1*, 1978, 1126 (*synth*)
Rice, C.R. *et al*, *Acta Cryst. C*, 1992, **48**, 1988 (*cryst struct*)

3,3′-Dinitro-2,4′-bipyridine, D-1-00480

9CI
[81330-16-7]
$C_{10}H_6N_4O_4$ M 246.1
Light-sensitive cryst. (MeOH). Mp 112-114.5°.

MacBride, J.A.H. *et al*, *Tet. Lett.*, 1981, **22**, 4545 (*synth*)

3,3′-Dinitro-4,4′-bipyridine, D-1-00481

9CI
[54356-26-2]
$C_{10}H_6N_4O_4$ M 246.1
Cryst. (EtOH). Mp 127-128°.

Kanoktanaporn, S. *et al*, *J.C.S. Perkin 1*, 1978, 1126 (*synth, ir, uv*)

4,4′-Dinitro-2,2′-bipyridine, D-1-00482

9CI
[18511-72-3]
$C_{10}H_6N_4O_4$ M 246.1
Cryst. (CH_2Cl_2/hexanes). Mp 190-192°.

N-*Oxide:* [84175-12-2].
$C_{10}H_6N_4O_5$ M 262.1 Cryst. (CH_2Cl_2). Mp 215-216.5°.

N,N′-*Dioxide:* [51595-55-2].
$C_{10}H_6N_4O_6$ M 278.1 Cryst. Mp 261° dec.

Murase, H. *et al*, *Nippon Kagaku Zasshi*, 1956, **77**, 682; *CA*, **52**, 9100a (*synth*)
Wenkert, D. *et al*, *J.O.C.*, 1983, **48**, 283 (*synth, uv, pmr*)
Wong, Y. *et al*, *Inorg. Chem.*, 1994, **33**, 1354 (*synth, pmr, cmr, dioxide*)

4,4′-Dinitro-3,3′-bipyridine, D-1-00483

9CI
[97033-23-3]
$C_{10}H_6N_4O_4$ M 246.1
Cryst. (MeOH). Mp 176-177°.

Kanoktanaporn, S. *et al*, *J. Chem. Res., Miniprint*, 1986, 2049 (*synth, uv, pmr*)

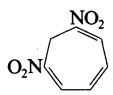
5,5′-Dinitro-2,2′-bipyridine, D-1-00484

9CI
[39858-84-9]
$C_{10}H_6N_4O_4$ M 246.1
Cryst. (Me_2CO). Mp 244-245°.

Case, F.H., *J.A.C.S.*, 1946, **68**, 2574 (*synth*)

1,6-Dinitro-1,3,5-cycloheptatriene, 9CI D-1-00485

[156545-34-5]



$C_7H_6N_2O_4$ M 182.1
Cryst. Mp 120-122°.

Burnett, I.J. *et al*, *Chem. Comm.*, 1994, 1187 (*synth, cryst struct, pmr, cmr*)

1,1-Dinitroethylene D-1-00486

1,1-Dinitroethene, 9CI
[34238-14-7]

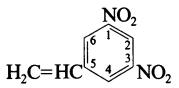
$H_2C{=}C(NO_2)_2$

$C_2H_2N_2O_4$ M 118.0
Reactive intermediate. Not isol. Formed from 1,1,1-Trinitroethane, T-0-06148 + base.

Zeldin, L. *et al*, *J.A.C.S.*, 1957, **79**, 4708.

1,3-Dinitro-5-vinylbenzene D-1-00487

1-Ethenyl-3,5-dinitrobenzene, 9CI. 3,5-Dinitrostyrene, 8CI. (3,5-Dinitrophenyl) ethylene
[72918-18-4]



$C_8H_6N_2O_4$ M 194.1

Japan. Pat., 01 204 931, (1989); *CA*, **112**, 159992c (*synth*)
Nagase, Y. *et al*, *Makromol. Chem. Rapid Commun.*, 1990, **11**, 185; *CA*, **113**, 41484f (*synth*)

Dioctyl disulfide, 9CI D-1-00488

[822-27-5]

$H_3C(CH_2)_7SS(CH_2)_7CH_3$

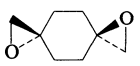
$C_{16}H_{34}S_2$ M 290.5
Oil. Bp_{13} 198-203°. n_D^{20} 1.4858.

S,S,S′,S′-*Tetraoxide: Dioctyl disulfone, 9CI*
$C_{16}H_{34}O_4S_2$ M 354.5 Plates (hexane). Mp 89.2-89.8°.

Westlake, H.E. *et al*, *J.A.C.S.*, 1942, **64**, 149 (*synth*)
Allen, P. *et al*, *J.O.C.*, 1951, **16**, 767 (*disulfone*)
Bruin, P. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1952, **71**, 1115 (*synth*)
Chorbadjiev, S. *et al*, *J. Prakt. Chem.*, 1977, **319**, 1036 (*synth*)
Zhang, Y. *et al*, *Synth. Commun.*, 1994, **24**, 2893 (*synth, pmr*)

1,7-Dioxadispiro[2.2.2.2] decane, 9CI, 8CI D-1-00489

1,4-Dimethylenecyclohexane dioxide
[184-83-8]



(3*RS*,6*RS*)-*form*

$C_8H_{12}O_2$ M 140.1

(***3RS,6RS*)-*form*** [28250-09-1]
trans-*form*
Cryst. (C_6H_6). Mp 106-107°.

(***3RS,6SR*)-*form*** [28250-28-4]
cis-*form*
Cryst. (C_6H_6). Mp 82°.

Causa, A.G. *et al*, *J.O.C.*, 1973, **38**, 1385 (*synth, ir, pmr*)
Becker, M. *et al*, *Chem. Ber.*, 1975, **108**, 2391 (*synth, ms, pmr*)

1,5,2,4-Dioxadithiepane, 9CI D-1-00490

$C_3H_6O_2S_2$ M 138.2

S,S,S′,S′-*Tetraoxide:* [99591-73-8]. *Cyclodisone. NSC 348948*
$C_3H_6O_6S_2$ M 202.2 Antineoplastic agent. Cryst. (cyclohexane/CH_2Cl_2). Mp 170°.

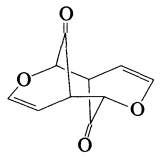
▶ LD_{50} (mus, orl) 253 mg/kg. JG7882000.

[100085-85-6]

Pat. Coop. Treaty (WIPO), 85 03 075, (1985); *CA*, **104**, 19609t (*Ciclodisone, synth*)
Gibson, N.W. *et al*, *Cancer Res.*, 1986, **46**, 1679 (*Ciclodisone, pharmacol*)
Berardini, M.D. *et al*, *Anti-Cancer Drug Des.*, 1991, **7**, 119 (*sar*)

3,8-Dioxatricyclo[5.3.1.1^{2,6}]dodeca-4,9-diene-11,12-dione, 9CI D-1-00491

[93517-46-5]



$C_{10}H_8O_4$ M 192.1
Pyrolysis prod. of cellulose. Pink rods (Me_2CO). Mp 165-168°.

Fumeaux, R.H. *et al*, *J.C.S. Perkin 1*, 1984, 1923 (*synth*)
Gainsford, G.J. *et al*, *Acta Cryst. C*, 1995, **51**, 1369 (*cryst struct*)

7,12-Dioxo-8,10-octadecadienoic acid D-1-00492

$H_3C(CH_2)_5COCH{=}CHCH{=}CHCO(CH_2)_5COOH$

$C_{18}H_{28}O_4$ M 308.4
(E,E)-form [110187-19-4] ***Ostopanic acid***
From fruit and stems of *Ostodes paniculata*. Inhibits growth of P-388 lymphocytic leukaemia test system *in vitro*. Cryst. Mp 122-123° (natural), Mp 132-133° (synthetic).

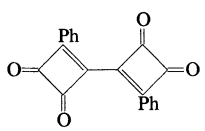
Et ester: [122947-35-7].
$C_{20}H_{32}O_4$ M 336.4 Cryst. Mp 87-88°.

Hamburger, M. *et al*, *J. Nat. Prod.*, 1987, **50**, 281 (*isol, pharmacol, pmr*)
Shen, J.H. *et al*, *J.O.C.*, 1989, **54**, 5126 (*synth, uv, ir, pmr, cmr, ms*)
Babudri, F. *et al*, *J.O.C.*, 1991, **56**, 6245 (*synth*)
Guo, C. *et al*, *J.C.S. Perkin 1*, 1993, 1921.
Bhalerao, U.T. *et al*, *Synth. Commun.*, 1993, **23**, 2213 (*synth, bibl*)

2,2′-Diphenyl[bi-1-cyclobuten-1-yl]-3,3′,4,4′-tetrone, 9CI D-1-00493

Bi(3-phenyl-3-cyclobutene-1,2-dione)

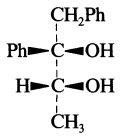
[152931-79-8]



$C_{20}H_{10}O_4$ M 314.2
Red cryst. (CH_2Cl_2). Mp 150° dec. Solns. dec. in air.

Liebeskind, L.S. *et al*, *J.A.C.S.*, 1993, **115**, 9048 (*synth, pmr, cmr*)

1,2-Diphenyl-2,3-butanediol, 9CI D-1-00494



(*2RS,3RS*)-*form*

$C_{16}H_{18}O_2$ M 242.3
(2RS,3RS)-form [87258-95-5]
Cryst. (petrol). Mp 78-79° (73-74°).
(2RS,3SR)-form [87258-96-6]
Mp 59-60°.

Chantrapromma, K. *et al*, *J.C.S. Perkin 1*, 1983, 1049 (*synth, pmr*)
Bach, T., *Annalen*, 1995, 1045 (*synth, ir, pmr, cmr, ms*)

1,4-Diphenyl-1-buten-3-yne D-1-00495

1,1′-(1-Buten-3-yne-1,4-diyl)bisbenzene, 9CI

PhCH=CHC≡CPh

$C_{16}H_{12}$ M 204.2
(E)-form [13343-79-8]
Cryst. (EtOH). Mp 96-97°.
(Z)-form [13343-78-7]
Pale yellow oil. Readily isomerises to (*E*)-form.

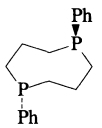
Straus, F., *Annalen*, 1905, **342**, 190 (*synth*)
Marcuzzi, F. *et al*, *J.C.S. Perkin 1*, 1993, 2957 *synth, ir, pmr*)

5,5-Diphenyl-2-cyclopenten-1-ol D-1-00496

$C_{17}H_{16}O$ M 236.3
(±)-form
Powder. Mp 50-55°.

Taniguchi, K. *et al*, *Chem. Pharm. Bull.*, 1995, **43**, 71 (*synth, pmr*)

1,5-Diphenyl-1,5-diphosphocane D-1-00497



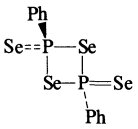
(1*RS*,5*RS*)-*form*

$C_{18}H_{22}P_2$ M 300.3
(1RS,5RS)-form [125707-15-5]
trans-*form*
Cryst. (EtOH). Mp 70-73°, Mp 74-76.5°.
1,5-Dioxide: [125707-18-8].
Solid. Mp 220-222°, Mp 229-231°.
(1RS,5SR)-form [125707-14-4]
cis-*form*
Solid. Mp 76-78°.
1,5-Dioxide: [125707-17-7].
$C_{18}H_{22}O_2P_2$ M 332.3 Solid. Mp 209-211°, Mp 214-215°.

Brooks, P.J. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1989, **44**, 235 (*synth, dioxide, uv, ir, P-31 nmr*)
Toto, S.D. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **56**, 27 (*synth, ir, ms, pmr, cmr, P-31 nmr, cryst struct*)
Musker, W.K., *Coord. Chem. Rev.*, 1992, **117**, 133 (*complexes, rev*)

2,4-Diphenyl-1,3,2,4-diselenadiphosphetane 2,4-diselenide D-1-00498

[122039-27-4]



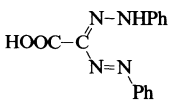
$C_{12}H_{10}P_2Se_4$ M 531.9
(1RS,3RS)-form [120875-49-2]
trans-*form*
Red solid.

Wood, P.T. *et al*, *Chem. Comm.*, 1988, 1190 (*synth, P-31 nmr, Se-77 nmr*)
Wood, P.T. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1989, **41**, 51 (*synth, ir, ms*)
Parkin, I.P. *et al*, *Polyhedron*, 1990, **9**, 987 (*synth, complexes*)

1,5-Diphenyl-3-formazancarboxylic acid, 9CI D-1-00499

(*Phenylazo*)(*phenylhydrazono*)*acetic acid, 8CI*

[1967-52-8]



$C_{14}H_{12}N_4O_2$ M 268.2
Red needles (EtOH). Mp 164° dec.

Me ester:
$C_{15}H_{14}N_4O_2$ M 282.3 Red needles (MeOH). Mp 134-135°.

Et ester: [6165-66-8].
$C_{16}H_{16}N_4O_2$ M 296.3 Prisms or leaflets (EtOH). Mp 117.5°.

Amide: [69211-06-9].
$C_{14}H_{13}N_5O$ M 267.2 Red cryst. (EtOH/AcOH). Mp 195-196°.

Nitrile: [7014-08-6]. *1,5-Diphenyl-3-formazancarbonitrile. 3-Cyano-1,5-diphenylformazan*
$C_{14}H_{11}N_5$ M 249.2 Bronze plates (EtOH or AcOH). Mp 161-162°.

v. Pechmann, H., *Ber.*, 1892, **25**, 3175 (*synth, esters*)
Bamberger, E. *et al*, *J. Prakt. Chem.*, 1902, **65**, 127 (*synth*)
Le Bris, M.-T. *et al*, *C. R. Hebd. Seances Acad. Sci.*, 1955, **241**, 1143 (*synth*)
Ishidate, M. *et al*, *Chem. Pharm. Bull.*, 1955, **3**, 224 (*nitrile*)
Dubenko, R.G. *et al*, *Zh. Org. Khim.*, 1978, **14**, 2112; *J. Org. Chem. USSR (Engl. Transl.)*, 1978, **14**, 1956 (*amide*)
Magdesieva, N.N. *et al*, *Zh. Org. Khim.*, 1983, **19**, 666; *J. Org. Chem. USSR (Engl. Transl.)*, 1983, **19**, 585 (*Et ester*)
Kolodina, T.S. *et al*, *Zh. Org. Khim.*, 1984, **20**, 661; *J. Org. Chem. USSR (Engl. Transl.)*, 1984, **20**, 601 (*amide*)

Zaitsev, B.E. *et al*, *Zh. Obshch. Khim.*, 1985, **55**, 1580; *J. Gen. Chem. USSR (Engl. Transl.)*, 1985, **55**, 1405 (*uv*)
Katritzky, A.R. *et al*, *Synthesis*, 1995, 577 (*amide*)

1,1-Diphenyl-1,5-hexadiene D-1-00500

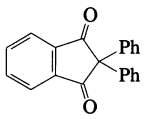
$Ph_2C{=}CHCH_2CH_2CH{=}CH_2$

$C_{18}H_{18}$ M 234.3
Oil.

Araki, S. *et al*, *J.C.S. Perkin 1*, 1995, 549 (*synth, ir, pmr, cmr*)

2,2-Diphenyl-1,3-indanedione, 8CI D-1-00501

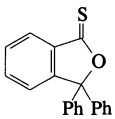
2,2-Diphenyl-1H-indene-1,3-(2H)-dione, 9CI
[23717-59-1]



$C_{21}H_{14}O_2$ M 298.3
Cryst. (EtOH or by subl.); needles (petrol). Mp 124-125° (118°).
2,4-Dinitrophenylhydrazone: Orange needles (EtOH). Mp 130°.

Moubasher, R. *et al*, *J.A.C.S.*, 1951, **73**, 3245 (*synth*)
Beringer, F.M. *et al*, *J.A.C.S.*, 1962, **84**, 2819 (*synth, uv*)
Agranat, I. *et al*, *Isr. J. Chem.*, 1969, **7**, 109 (*pmr*)
Schönberg, A. *et al*, *Chem. Ber.*, 1973, **106**, 849 (*synth, pmr*)
Watanabe, M. *et al*, *Synthesis*, 1994, 1083 (*synth, uv, pmr*)

3,3-Diphenyl-1(3*H*)-isobenzofuranthione D-1-00502



$C_{20}H_{14}OS$ M 302.3
Cryst. Mp 133-134°.

Nishio, T., *J.C.S. Perkin 1*, 1995, 561 (*synth, ir, pmr, cmr*)

N-(Diphenylmethylene)aniline D-1-00503

N-(*Diphenylmethylene*)*benzenamine, 9CI. N-Phenylbenzhydrylidenimine. Benzophenone phenylimine*
[574-45-8]

$Ph_2C{=}NPh$

$C_{19}H_{15}N$ M 257.3
Cryst. (hexane or EtOH). Mp 116-117°.
Hydrochloride: [23285-75-8]. Yellow cryst. Mp 190°.
Hydroiodide: Yellow cryst. Mp 185° dec.
Methiodide: Yellow cryst. Mp 202°.

Dimroth, O. *et al*, *Ber.*, 1902, **35**, 984 (*synth*)
Graebe, C. *et al*, *Ber.*, 1902, **35**, 2615 (*synth*)
Schonberg, A. *et al*, *J.C.S.*, 1935, 530 (*synth*)
Ruxer, J.M. *et al*, *Org. Magn. Reson.*, 1977, **10**, 105 (*conformn*)
Allen, M. *et al*, *Can. J. Chem.*, 1981, **59**, 451 (*cmr*)
Kosugi, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 677 (*synth*)
Baliah, V. *et al*, *J. Indian Chem. Soc.*, 1989, **66**, 42 (*ir*)
Strekowski, L. *et al*, *J.O.C.*, 1989, **54**, 6120 (*synth, pmr*)

(Diphenylmethyl)phosphonic acid D-1-00504

Benzhydrylphosphonic acid
[92025-81-5]

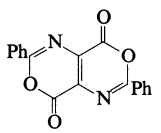
$Ph_2CHP(O)(OH)_2$

$C_{13}H_{13}O_3P$ M 248.2
Solid. Mp 237-239°.
Di-Me ester: [54963-39-2]. *Dimethyl (diphenylmethyl)phosphonate*
$C_{15}H_{17}O_3P$ M 276.2 Cryst. (cyclohexane). Mp 95-96°.
Di-Et ester: [27329-60-8]. *Diethyl (diphenylmethyl)phosphonate*
$C_{17}H_{21}O_3P$ M 304.3 Cryst. (cyclohexane). Mp 27-28.5°, Mp 40-41°.
Diisopropyl ester: [27329-62-0]. *Diisopropyl (diphenylmethyl)phosphonate*
$C_{19}H_{25}O_3P$ M 332.3 Cryst. (cyclohexane). Mp 80-81°.
Di-tert-butyl ester: Bis(1,1-dimethylethyl) (diphenylmethyl)phosphonate
$C_{21}H_{29}O_3P$ M 360.4 Cryst. (petrol). Mp 145-146° dec.

Poshkus, A.C. *et al*, *J.O.C.*, 1964, **29**, 2567 (*synth*)
Polozov, A.M. *et al*, *Synthesis*, 1990, 515 (*synth, pmr, P-31 nmr*)
Polozov, A.M. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1992, **73**, 153 (*ester, synth, pmr, P-31 nmr*)
Ha, C. *et al*, *J.O.C.*, 1993, **58**, 1194 (*ester, synth, pmr, cmr*)
Polozov, A.M. *et al*, *Zh. Obshch. Khim.*, 1993, **63**, 229; *J. Gen. Chem. USSR (Engl. Transl.)*, 1993, **63**, 169 (*ester, synth, ir, pmr, P-31 nmr*)

2,6-Diphenyl[1,3]oxazino[5,4-*d*][1,3]oxazine-4,8-dione, 9CI D-1-00505

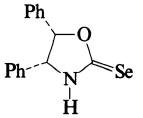
Hippuroflavine
[72884-73-2]



$C_{18}H_{10}N_2O_4$ M 318.2
Obt. from *N*-Benzoylglycine, B-0-01282. Yellow cryst. (diphenyl ether). Mp >310° dec.

Stachel, H.-D. *et al*, *Arch. Pharm. (Weinheim, Ger.)*, 1979, **312**, 968 (*synth, cryst struct*)

4,5-Diphenyl-2-oxazolidineselone, 9CI D-1-00506



$C_{15}H_{13}NOSe$ M 302.2

(4S,5R)-form [136794-55-3]
(+)-cis-*form*
Cryst. Mp 155-158°. $[\alpha]_D$ +68.7 (c, 0.18 in $CHCl_3$).

Peng, J. *et al*, *J.O.C.*, 1994, **59**, 4977 (*synth, uv, ir, pmr, cmr, Se-77 nmr*)

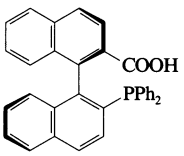
Diphenylphosphinecarboxylic acid D-1-00507

Ph_2PCOOH

$C_{13}H_{11}O_2P$ M 230.2
Solid (as Na salt or Li). Mp 235-240° (Na salt) and >250° (Li salt).
Me ester: [70533-07-2]. *Methyl diphenylphosphinecarboxylate*
$C_{14}H_{13}O_2P$ M 244.2 Ligand for Pt. Liq. $Bp_{0.1}$ 169-171°.
Trimethylsilyl ester: Trimethylsilyl diphenylphosphinecarboxylate
$C_{16}H_{19}O_2PSi$ M 302.3 Oil. n_D^{23} 1.5665.
Anilide: see *N,1,1-Triphenylphosphinecarbonamide, T-0-06398*
[18789-77-0, 120175-90-8, 154498-88-1]

Abel, E.W. *et al*, *J.C.S.(A)*, 1968, 1105 (*silyl ester*)
Duane Dombek, B., *J. Organomet. Chem.*, 1979, **169**, 315 (*ester, synth, ir, pmr, complex*)
Horn, H.-G. *et al*, *Chem.-Ztg.*, 1988, **112**, 195 (*silyl ester, pmr, cmr, Si-29 nmr, P-31 nmr*)
Diemert, K. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **60**, 287; 1993, **83**, 65 (*synth, derivs, ir, pmr, P-31 nmr*)

2′-(Diphenylphosphino)-[1,1′-binaphthalene]-2-carboxylic acid, 9CI D-1-00508



(*R*)-*form*

$C_{33}H_{23}O_2P$ M 482.5
(R)-form [156456-75-6]
Solid. Mp 124-126°. $[\alpha]_D^{20}$ +65.9 (c, 0.54 in $CHCl_3$).
Me ester: [156456-74-5].
$C_{34}H_{25}O_2P$ M 496.5 Solid. Mp 105-108°. $[\alpha]_D^{20}$ +42.0 (c, 0.52 in $CHCl_3$).
Me ester, P-oxide: [156456-73-4].
$C_{34}H_{25}O_3P$ M 512.5 Solid. Mp 174-176°. $[\alpha]_D^{20}$ +41.5 (c, 0.57 in $CHCl_3$).
Nitrile: [156456-69-8].
$C_{33}H_{22}NP$ M 463.5 Solid. Mp 143-144°. $[\alpha]_D^{20}$ +57.6 (c, 0.53 in $CHCl_3$).
Nitrile, oxide: [156456-68-7].
$C_{33}H_{22}NOP$ M 479.5 Solid. Mp 212-214°. $[\alpha]_D^{20}$ +132.1 (c, 0.49 in $CHCl_3$).

Uozumi, Y. *et al*, *Tetrahedron*, 1994, **50**, 4293 (*synth, ir, ms, pmr, P-31 nmr*)

(Diphenylphosphinodithioato) phenyltellurium(*II*) D-1-00509

Phenyltellurium diphenyldithiophosphinate. Phenyltellurium diphenylphosphinodithioate. Diphenylphosphino(tellurothioperoxo)thioic acid, 9CI
[153632-71-4]

$Ph_2P(S)STePh$

$C_{18}H_{15}PS_2Te$ M 454.0
Red prismatic cryst. Thermochromic; becomes yellow at −60°.

Silvestra, A. *et al*, *Inorg. Chem.*, 1994, **33**, 1253 (*synth, cryst struct*)

P-[2-(Diphenylphosphino)ethyl]-*N,N,N',N'*-tetramethylphosphonous diamide D-1-00510

[2-(*Diphenylphosphino*)*ethyl*]*phosphonous bis*(*dimethylamide*)

[36892-72-5]

$Ph_2PCH_2CH_2P(NMe_2)_2$

$C_{18}H_{26}N_2P_2$ M 332.3
Ligand. Thick liq. $Bp_{0.005}$ 146-158°. Easily oxidised.

King, R.B. *et al*, *J.A.C.S.*, 1977, **99**, 4001 (*synth, pmr, cmr, P-31 nmr*)

3-(Diphenylphosphino)pyridine D-1-00511

Diphenyl-3-pyridinylphosphine

[104114-99-0]

$C_{17}H_{14}NP$ M 263.2
Ligand for Mo and Pd. Complexes of use in the carbonylation of alkynes. Flaky cryst.

Lazarowych, N.J. *et al*, *Inorg. Chem.*, 1986, **25**, 3926.
Drent, E. *et al*, *J. Organomet. Chem.*, 1993, **455**, 247; 1994, **475**, 57 (*complexes, use*)

2-(Diphenylphosphino)-1,1,3,3-tetraphenyltriphosphine, 9CI, 8CI D-1-00512

Tris(*diphenylphosphino*)*phosphine*

[18005-88-4]

$P(PPh_2)_3$

$C_{36}H_{30}P_4$ M 586.5
Ligand for Cr, Mo and W. Cryst. (Et_2O). Mp 118-120°.

Schumann, H. *et al*, *J. Organomet. Chem.*, 1970, **24**, 183 (*synth, ir, Raman*)
Scheer, M. *et al*, *Z. Anorg. Allg. Chem.*, 1991, **600**, 203; 1993, **619**, 1047 (*synth, ms, P-31 nmr*)

2,3-Diphenyl-1,2-propanediol, 9CI D-1-00513

[155203-78-4]

$PhCH_2CPh(OH)CH_2OH$

$C_{15}H_{16}O_2$ M 228.2
(±)-*form* [157008-56-5]
Needles (Et_2O/petrol). Mp 77-78° (73°).

Ramart-Lucas, M. *et al*, *Bull. Soc. Chim. Fr.*, 1932, **51**, 1069 (*synth*)
Freudenberg, K. *et al*, *Chem. Ber.*, 1952, **85**, 78 (*synth*)
Bach, T., *Annalen*, 1995, 1045 (*synth, ir, pmr, cmr, ms*)

1,3-Diphenyl-3-propen-1-ol, 8CI D-1-00514

α-(*2-Phenylethenyl*)*benzenemethanol, 9CI. Chalcol*

[4663-33-6]

$PhCH(OH)CH{=}CHPh$

$C_{15}H_{14}O$ M 210.2
(±)-(*E*)-*form* [62668-02-4]
Cryst. (petrol). Mp 55-56°.
(±)-(*Z*)-*form* [62839-70-7]
Liq. $Bp_{1.3}$ 147-150°.

[73930-97-9, 87751-69-7, 116127-91-4, 124150-25-0, 132014-29-0, 136981-81-2, 148616-45-9]

Wasserman, H.H. *et al*, *J.A.C.S.*, 1955, **77**, 590 (*synth*)
Neumann, H. *et al*, *Chem. Ber.*, 1978, **111**, 2785 (*synth, ir, pmr*)
Takai, K. *et al*, *Tet. Lett.*, 1983, **24**, 5281 (*synth*)

2,5-Diphenyl-3-pyridinecarboxylic acid D-1-00515

2,5-Diphenylnicotinic acid

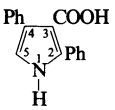
$C_{18}H_{13}NO_2$ M 275.3

Amide:
$C_{18}H_{14}N_2O$ M 274.3 Cryst. (EtOH). Mp 223-225°.

Nitrile: [156020-89-2]. *3-Cyano-2,5-diphenylpyridine*
$C_{18}H_{12}N_2$ M 256.3 Cryst. (EtOH). Mp 132°.

Kagabu, S. *et al*, *J.C.S. Perkin 1*, 1994, 739.

2,4-Diphenyl-1*H*-pyrrole-3-carboxylic acid, 9CI D-1-00516



$C_{17}H_{13}NO_2$ M 263.2

Me ester: [59009-61-9].
$C_{18}H_{15}NO_2$ M 277.3 Cryst. (CH_2Cl_2/Et_2O/pentane). Mp 164.5-165.5°.

Et ester: [63324-78-7].
$C_{19}H_{17}NO_2$ M 291.3 Mp 106°.

Nitrile: [59009-62-0]. *3-Cyano-2,4-diphenylpyrrole*
$C_{17}H_{12}N_2$ M 244.2 Cryst. (Me_2CO). Mp 280° (266-267°).

Filho, P.F.D.S. *et al*, *Angew. Chem.*, 1977, **89**, 672 (*nitrile, Et ester*)
Houwing, H.A. *et al*, *J. Het. Chem.*, 1981, **18**, 1127 (*nitrile, Me ester*)

2,5-Diphenyl-1*H*-pyrrole-3-carboxylic acid, 9CI D-1-00517

[93325-15-6]

$C_{17}H_{13}NO_2$ M 263.2
Prisms (EtOH aq.). Mp 207-208° (200°).

Me ester: [13901-74-1].
$C_{18}H_{15}NO_2$ M 277.3 Cryst. (MeOH). Mp 172-173° (162°).

Et ester: [65474-26-2].
$C_{19}H_{17}NO_2$ M 291.3 Prisms (EtOH). Mp 160-161° (150-154°).

Nitrile: [67421-66-3]. *3-Cyano-2,5-diphenylpyrrole*
$C_{17}H_{12}N_2$ M 244.2 Cryst. (C_6H_6 or EtOH). Mp 228-230° (218.5-219.5°). Change in crystalline form at 190°.

N-*Me:* [130850-55-4].
$C_{18}H_{15}NO_2$ M 277.3 Mp 213-214°.

N-*Ph:* [130850-56-5]. *1,2,5-Triphenyl-1H-pyrrole-3-carboxylic acid*
$C_{23}H_{17}NO_2$ M 339.3 Mp 278-279°.

Henze, H.R. *et al*, *J.A.C.S.*, 1947, **69**, 1662 (*nitrile*)
Sprio, V. *et al*, *Ann. Chim.* (*Rome*), 1960, **50**, 1635 (*Et ester*)
Bayer, H.O. *et al*, *Chem. Ber.*, 1970, **103**, 2356 (*Me ester*)
Benages, I.A. *et al*, *J.O.C.*, 1978, **43**, 4273 (*nitrile*)
Petruso, S. *et al*, *J. Het. Chem.*, 1990, **27**, 1277 (*synth, pmr, ir*)

3,4-Diphenyl-1*H*-pyrrole-2-carboxylic acid, 9CI D-1-00518

$C_{17}H_{13}NO_2$ M 263.2

Me ester: [151054-89-6].
$C_{18}H_{15}NO_2$ M 277.3 Cryst. (MeOH aq.). Mp 125-126°.

Rolfs, A. *et al*, *Angew. Chem., Int. Ed.*, 1993, **32**, 712 (*Me ester*)

3,5-Diphenyl-1*H*-pyrrole-2-carboxylic acid, 9CI D-1-00519

[100784-98-3]

$C_{17}H_{13}NO_2$ M 263.2
Mp 180°.

Me ester: [89649-52-5].
$C_{18}H_{15}NO_2$ M 277.3 Cryst. (MeOH). Mp 179°.

Et ester: [53778-26-0].
$C_{19}H_{17}NO_2$ M 291.3 Prisms (hexane). Mp 142° (135-137°).

Nitrile: [131475-18-8]. *2-Cyano-3,5-diphenylpyrrole*
$C_{17}H_{12}N_2$ M 244.2 Mp 195-196°.

Mataka, S. *et al*, *Synthesis*, 1982, 157 (*Et ester*)
Sammes, M.P. *et al*, *J.C.S. Perkin 1*, 1985, 1773 (*Et ester, Me ester, ir, pmr*)
Alberola, A. *et al*, *Heterocycles*, 1990, **31**, 1049 (*Et ester, nitrile*)

4,5-Diphenyl-1*H*-pyrrole-3-carboxylic acid, 9CI D-1-00520

[161958-67-4]

$C_{17}H_{13}NO_2$ M 263.2
Mp 223-225° dec.

Me ester: [40167-39-3].
$C_{18}H_{15}NO_2$ M 277.3 Cryst. (C_6H_6/cyclohexane). Mp 184-185°.

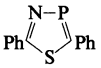
Et ester: [73799-68-5].
$C_{19}H_{17}NO_2$ M 291.3 Cryst. (C_6H_6/cyclohexane). Mp 207-208.5° (191-193°).

Nitrile: [161958-65-2]. *4-Cyano-2,3-diphenylpyrrole*
$C_{17}H_{12}N_2$ M 244.2 Cryst. (C_6H_6/cyclohexane). Mp 139-141°.

van Leusen, A.M. *et al*, *Tet. Lett.*, 1972, 5337 (*Me ester*)
Di Santo, R. *et al*, *Synth. Commun.*, 1995, **25**, 795 (*synth, Me ester, Et ester, nitrile*)

2,5-Diphenyl-1,3,4-thiazphosphole D-1-00521

[94570-25-9]

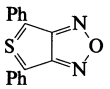


$C_{14}H_{10}NPS$ M 255.2
Cryst. Mp 85-87°. Stable to oxidn., but sensitive to hydrolysis.

Schmidpeter, A. *et al*, *Angew. Chem., Int. Ed.*, 1985, **24**, 123 (*synth, cmr, P-31 nmr, props, cryst struct*)

4,6-Diphenylthieno[3,4-*c*]-1,2,5-oxadiazole-5-*S*^{IV} D-1-00522

[64959-93-9]



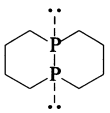
$C_{16}H_{10}N_2OS$ M 278.3
Blue cryst. Mp 161-165° dec.

Tsuge, O. *et al*, *Heterocycles*, 1977, **6**, 1173 (*synth*)

1,6-Diphosphabicyclo[4.4.0]decane D-1-00523

Octahydro[1,2]diphosphorino[1,2-a][1,2]diphosphorin

[144909-28-4]



$C_8H_{16}P_2$ M 174.1

(*1RS,6SR*)-*form* [144654-28-4]
cis-*form*
Stable at 300° for 4h; some dec. at 400°. Possesses double chair conform.

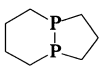
[144654-36-4]

Alder, R.W. *et al*, *Chem. Comm.*, 1992, 1170 (*synth, cryst struct, P-31 nmr*)

1,6-Diphosphabicyclo[4.3.0]nonane D-1-00524

Hexahydro-1H-[1,2]diphospholo[1,2-a][1,2]diphosphorin

[117440-57-0]

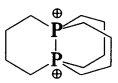


$C_7H_{14}P_2$ M 160.1
Phys. props. not reported.

Alder, R.W. *et al*, *Chem. Comm.*, 1992, 1170 (*synth, P-31 nmr*)

1,6-Diphosphatricyclo[4.4.4.0]tetradecanediium(2+) D-1-00525

Octahydro-5,10-butano[1,2]diphosphorino[1,2-a][1,2]diphosphorindiium(2+), 9CI. 1,6-Diphosphonia[4.4.4]propellane



$C_{12}H_{24}P_2^{2\oplus}$ M 230.2 (ion)
Bis(trifluoromethanesulfonate): [144909-30-8].
$C_{14}H_{24}F_6O_6P_2S_2$ M 528.4 Cryst.

Alder, R.W. *et al*, *Chem. Comm.*, 1992, 1172 (*synth, P-31 nmr, cryst struct*)

N,N'-Di-2-propenylurea D-1-00526

1,3-Diallylurea. Sinapolin

[1801-72-5]

$H_2C{=}CHCH_2NHCONHCH_2CH{=}CH_2$

$C_7H_{12}N_2O$ M 140.1
Intermed. for hetereocyclic synth. Plates. Mp 90-93°.

Will, H., *Annalen*, **52**, 27.
Cahours, A. *et al*, *Annalen*, 1857, **102**, 300.

Dipropyl diselenide, 9CI D-1-00527

Propyl diselenide, 8CI

[7361-89-9]

$H_3CCH_2CH_2SeSeCH_2CH_2CH_3$

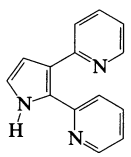
$C_6H_{14}Se_2$ M 244.0
Orange liq. with offensive odour. Bp_{15} 103-104°.

Tschugaeff, L., *Ber.*, 1909, **42**, 49 (*synth, props*)
Backer, H.J. *et al*, *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1935, **54**, 531 (*synth*)
Cohen, V.I. *et al*, *J.O.C.*, 1977, **42**, 2510 (*synth*)
Gladysz, J.A. *et al*, *J.O.C.*, 1978, **43**, 1204 (*synth, pmr*)
Korchevin, N.A. *et al*, *Zh. Obshch. Khim.*, 1989, **59**, 1788; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1989, **59**, 1592 (*synth*)

2,3-Di-2-pyridinyl-1*H*-pyrrole D-1-00528

2,2'-(1H-Pyrrole-2,3-diyl)bispyridine, 9CI

[147821-73-6]

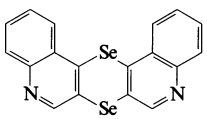


$C_{14}H_{11}N_3$ M 221.2
Oil.

Katritzky, A.R. *et al*, *J.O.C.*, 1994, **59**, 4551 (*synth, pmr, cmr*)

[1,4]Diselenino[2,3-*c*:6,5-*c'*]diquinoline, 9CI D-1-00529

[162469-50-3]



$C_{18}H_{10}N_2Se_2$ M 412.2
Needles (EtOH). Mp 279°.

Löwe, W. *et al*, *J. Het. Chem.*, 1995, **32**, 271 (*synth, pmr*)

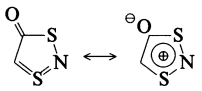
1,3,2-Dithiazol-1-ium(1+), 9CI D-1-00530

$C_2H_2NS_2^{\oplus}$ M 104.1 (ion)
Chloride: [139366-59-9].
$C_2H_2ClNS_2$ M 139.6 Hygroscopic solid. Mp >230° dec.

Gray, M.A. *et al*, *J.C.S. Perkin 1*, 1993, 3077 (*synth, ir, uv, pmr, N nmr*)

1,3,2-Dithiazol-4-one D-1-00531

4-Hydroxy-1,3,2-dithiazol-1-ium inner salt, 9CI

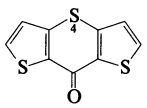


C_2HNOS_2 M 119.1
Unstable, golden-yellow oil.

Gray, M.A. *et al*, *J.C.S. Perkin 1*, 1993, 3077 (*synth, cmr, ms*)

8*H*-Dithieno[3,2-*b*:2',3'-*e*]thiopyran-8-one, 9CI D-1-00532

[3807-51-0]



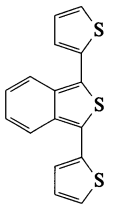
$C_9H_4OS_3$ M 224.3
Cryst. (EtOH). Mp 189-190.5°.

4-Oxide: [157368-13-3].
$C_9H_4O_2S_3$ M 240.3 Cryst. Mp 230-232° dec.

Stoyanovich, F.M. *et al*, *Zh. Org. Khim.*, 1965, **1**, 1282; *J. Org. Chem. USSR* (*Engl. Transl.*), 1965, **1**, 1296 (*synth*)
Suzuki, Y. *et al*, *Chem. Comm.*, 1994, 1431 (*sulfoxide, synth*)

1,3-Di-2-thienylbenzo[*c*]thiophene, 9CI D-1-00533

[144810-53-7]

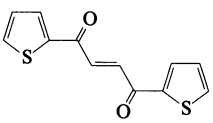


$C_{16}H_{10}S_3$ M 298.4
Forms an electroactive polymer. Orange cryst. Mp 100-102°.

Musmanni, S. *et al*, *Chem. Comm.*, 1993, 172 (*synth, uv, props*)

1,4-Di-2-thienyl-2-butene-1,4-dione, 9CI D-1-00534

[99971-34-3]



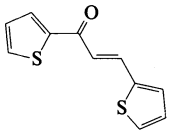
$C_{12}H_8O_2S_2$ M 248.3

(*E*)-*form* [13669-00-6]
Yellow needles. Mp 196-197° (188-189°).

Heffe, W. *et al*, *Chem. Ber.*, 1956, **89**, 822 (*synth*)
Kooreman, H.J. *et al*, *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1967, **86**, 37 (*synth, ir, uv, pmr*)

1,3-Di-2-thienyl-2-propen-1-one, 9CI D-1-00535

[2309-48-0]



$C_{11}H_8OS_2$ M 220.3
Mp 99-100°. Prob. (*E*)-form.

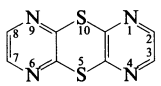
[42811-88-1]

Lavrushin, V.F. *et al*, *Khim. Geterotsikl. Soedin.*, 1971, **7**, 1361 (*uv*)
El-Rayyes, N.R., *J. Het. Chem.*, 1982, **19**, 415 (*synth, uv, ir, pmr*)
Matsui, M. *et al*, *J.C.S. Perkin 2*, 1992, 201 (*synth, pmr*)
Zhengdong, L. *et al*, *Acta Cryst. C*, 1995, **51**, 681 (*cryst struct*)

[1,4]Dithiino[2,3-*b*:5,6-*b'*] dipyrazine D-1-00536

1,4,6,9-Tetraazathianthrene

[52879-26-2]



$C_8H_4N_4S_2$ M 220.2
Yellow needles ($CHCl_3$).

Lynch, V.M. *et al*, *Acta Cryst. C*, 1994, **50**, 1470 (*cryst struct*)

2,2'-Dithiobis[2-methylpropanal], 9CI D-1-00537

2,2,5,5-Tetramethyl-3,4-dithia-1,6-hexanedial. α,α'-Dithiodiisobutyraldehyde

[15581-80-3]

$OHCC(CH_3)_2SSC(CH_3)_2CHO$

$C_8H_{14}O_2S_2$ M 206.3
Evil smelling oil or cryst. Bp_1 100-110°, $Bp_{0.06}$ 78°.

▶ Hazardous prepn. (toxic gases).

Dioxime:
$C_8H_{16}N_2O_2S_2$ M 236.3 Fine needles (EtOH). Mp 127°.

Bis(semicarbazone): Small cryst. (EtOH). Mp 218° dec.

Bis(phenylhydrazone): Needles (EtOH). Mp 156.5-157°.

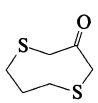
Bis(2,4-dinitrophenylhydrazone): Reddish yellow powder (DMF or EtOAc). Mp 217° dec.

Merz, K.W. *et al*, *Arch. Pharm. (Weinheim, Ger.)*, 1963, **296**, 427 (*synth, deriv*)
D'Amico, J.J. *et al*, *J.O.C.*, 1975, **40**, 1224 (*synth, pmr*)
Roy, B. *et al*, *J.O.C.*, 1994, **59**, 7019 (*synth, pmr, cmr, ir, haz*)

1,5-Dithiocan-3-one, 9CI D-1-00538

1,5-Dithia-3-cyclooctanone

[39958-62-8]

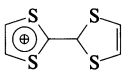


$C_6H_{10}OS_2$ M 162.2
Cryst. (EtOH). Mp 47°.

2,4-Dinitrophenylhydrazone: Solid (C_6H_6/hexane). Mp 180-182°.

Howard, E.G. *et al*, *J.A.C.S.*, 1960, **82**, 158 (*synth*)
Arya, V.P., *Indian J. Chem.*, 1972, **10**, 812 (*synth, uv, pmr*)
Kellogg, R.M. *et al*, *J.O.C.*, 1993, **58**, 5624 (*synth, pmr, cmr, ir*)
Meier, H. *et al*, *Chem. Ber.*, 1994, **127**, 2035 (*synth, pmr, cmr*)

2-(1,3-Dithiol-2-yl)-1,3-dithiol-1-ium(1+), 9CI D-1-00539



$C_6H_5S_4^{\oplus}$ M 205.3 (ion)
Protonated form of Tetrathiafulvalene, T-0-02747.

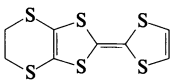
Tetrafluoroborate: [151516-16-4].
$C_6H_5BF_4S_4$ M 292.1 Dark-red fine needles (MeCN at −20°). Mp 195-200°. Reactive with H_2O.

Giffard, M. *et al*, *Chem. Comm.*, 1993, 944 (*synth, pmr, cmr, cryst struct*)

2-(1,3-Dithiol-2-ylidene)-5,6-dihydro-1,3-dithiolo[4,5-*b*][1,4]dithiin, 9CI D-1-00540

Ethylenedithiotetrathiafulvalene. EDT-TTF

[97307-49-8]



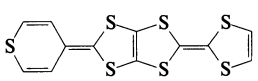
$C_8H_6S_6$ M 294.5
Forms superconductive salts. Red cryst. (CH_3CN/toluene). Mp 206-207°.

Papavassiliou, G.C. *et al*, *Mol. Cryst. Liq. Cryst.*, 1988, **156**, 269 (*synth, uv*)
Garreau, B. *et al*, *C. R. Hebd. Seances Acad. Sci. Ser. 2*, 1991, **313**, 509 (*synth, cryst struct*)
Orduna, J. *et al*, *Rapid Commun. Mass Spectrom.*, 1993, **7**, 815 (*ms*)
Formigué, M. *et al*, *Synthesis*, 1993, 509 (*synth*)

2-(1,3-Dithiol-2-ylidene)-5-(4*H*-thiopyran-4-ylidene)[1,3]dithiolo[4,5-*d*]-1,3-dithiole, 9CI D-1-00541

2-(1',3'-Dithiol-2-ylidene)-5-(thiopyran-4''-ylidene)-1,3,4,6-tetrathiapentalene. TPDT-TTP

[153916-43-9]

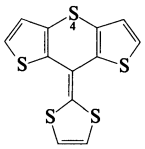


$C_{12}H_6S_7$ M 374.6
Forms conducting charge-transfer complexes. Orange, plate-like microcryst. Mp 200-201° dec.

Misaki, Y. *et al*, *Chem. Comm.*, 1993, 949 (*synth, pmr, props*)

8-(1,3-Dithiol-2-ylidene)-8*H*-dithieno[3,2-*b*:2',3'-*e*]thiopyran, 9CI D-1-00542

[157368-11-1]



$C_{12}H_6S_5$ M 310.5
Strong electron donor. Cryst. Mp 105-107° dec.

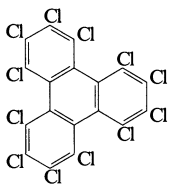
4-Oxide: [157368-16-6].
$C_{12}H_6OS_5$ M 326.5 Cryst. Mp 198-200° dec.

Suzuki, T. *et al*, *Chem. Comm.*, 1994, 1431 (*synth, use, pmr, uv*)

Dodecachlorotriphenylene D-1-00543

Perchlorotriphenylene

[137695-68-2]



$C_{18}Cl_{12}$ M 641.6
Mp 347-348°. Difficult to synthesise, highly distorted molecule. Exhaustive chlorination of Triphenylene, T-0-06330 causes rearrangement.

Shibata, K. *et al*, *J.A.C.S.*, 1994, **116**, 5983 (*synth, cryst struct*)

4,8-Dodecadiyn-1-ol D-1-00544

$H_3CCH_2CH_2C{\equiv}CCH_2CH_2C{\equiv}CCH_2CH_2CH_2OH$

$C_{12}H_{18}O$ M 178.2
Oil.

Bao, J. *et al*, *J.A.C.S.*, 1994, **116**, 7616 (*synth, ir, pmr, cmr, ms*)

5,10-Dodecadiyn-1-ol D-1-00545

[160109-68-2]

$H_3CC{\equiv}C(CH_2)_3C{\equiv}C(CH_2)_3CH_2OH$

$C_{12}H_{18}O$ M 178.2
Oil.

Bao, J. *et al*, *J.A.C.S.*, 1994, **116**, 7616 (*synth, ir, pmr, cmr, ms*)

1,1,2,2,3,3,4,4,5,5,6,6-Dodecafluoro-1,6-diiodohexane D-1-00546

1,6-Diiodoperfluorohexane

[375-80-4]

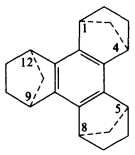
$ICF_2(CF_2)_4CF_2I$

$C_6F_{12}I_2$ M 553.8
d^{30} 2.36. Mp 25°. Bp_{100} 115°. n_D^{30} 1.3980.

Haszeldine, R.N., *J.C.S.*, 1953, 1764 (*uv*)

Knunyants, I.L. *et al*, *Izv. Akad. Nauk Kaz. SSR, Ser. Khim.*, 1964, 384; *CA*, **60**, 11883h (*synth*)

1,2,3,4,5,6,7,8,9,10,11,12-Dodecahydro[1,4:5,8:9,12]trimethanotriphenylene, 9CI D-1-00547



$C_{21}H_{24}$ M 276.4

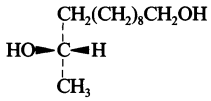
(1α,4α,5α,8α,9α,12α)-form [75599-41-6]
all-syn-*form*
Mp 175-180°.

(1α,4α,5α,8α,9β,12β)-form [75574-95-7]
syn-anti-syn-*form*
Mp 165-168°.

Gassman, P.G. *et al*, *J.A.C.S.*, 1980, **102**, 6863.

1,11-Dodecanediol D-1-00548

[80158-99-2]



(*S*)-*form*

$C_{12}H_{26}O_2$ M 202.3

(S)-form
Solid (Et_2O). Mp 40-42°. $[\alpha]_D^{24}$ +0.6 (c, 2.9 in $CHCl_3$).

(±)-form
11-Ac: [77413-19-5].
$C_{14}H_{28}O_3$ M 244.3 Bp_1 135°.

Asaoka, M. *et al*, *Tet. Lett.*, 1980, **21**, 4611 (*Ac*)
Enders, D. *et al*, *Annalen*, 1995, 1185 (*S-form, synth, ir, pmr, cmr, ms*)

3,6,9-Dodecatrienoic acid D-1-00549

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2COOH$

$C_{12}H_{18}O_2$ M 194.2

(all-Z)-form [92340-48-2]
Constit. of the female gametes of *Analipus japonicus*. Possible precursor of algal sex attractants.

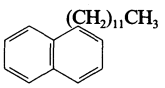
[82461-32-3]

Kodama, K. *et al*, *Phytochemistry*, 1993, **33**, 1039 (*isol, synth, pmr, cmr*)

1-Dodecylnaphthalene D-1-00550

1-(1-Naphthalenyl)dodecane

[26438-28-8]



$C_{22}H_{32}$ M 296.4
Fp 27°. Bp 415°, Bp_1 187°.

Adv. Chem. Ser., 1955, **15**, 236 (***props***)

2-Dodecylnaphthalene D-1-00551

1-(2-Naphthalenyl)dodecane

[60899-39-0]

$C_{22}H_{32}$ M 296.4
Bp 414°, Bp_1 187°.

Adv. Chem. Ser., 1955, **15**, 23 (***props***)

Dodecylphosphonic acid D-1-00552

[5137-70-2]

$H_3C(CH_2)_{11}P(O)(OH)_2$

$C_{12}H_{27}O_3P$ M 250.3
Solid. Mp 100.5-101.5°.

Di-Et ester: [4844-38-6]. *Diethyl dodecylphosphonate*
$C_{16}H_{35}O_3P$ M 306.4 Liq. Bp_1 160°. $n_D^{16.5}$ 1.4419.

Dibutyl ester: [5929-68-0]. *Dibutyl dodecylphosphonate*
$C_{20}H_{43}O_3P$ M 362.5 Liq. d_4^{25} 0.92. Bp_3 196-199°. n_D^{25} 1.4432.

Di-Ph ester: Diphenyl dodecylphosphonate
$C_{24}H_{35}O_3P$ M 402.5 Liq. $Bp_{0.01}$ 165°. n_D^{25} 1.5111.

Dichloride: [3586-98-9].
$C_{12}H_{25}Cl_2OP$ M 287.2 Liq. cryst. at <5°. d_4^{20} 1.05. $Bp_{0.3}$ 128-130°, $Bp_{0.1}$ 148-151°. n_D^{20} 1.4709.

[16693-57-5]

Kosolapoff, G.M., *J.A.C.S.*, 1945, **67**, 1180 (*synth*)
Ford-Mason, A.H. *et al*, *J.C.S.*, 1947, 1465 (*synth*)
Laughton, R.G., *J.O.C.*, 1962, **27**, 3644 (*diphenyl ester*)
Raskina, L.P. *et al*, *Zh. Prikl. Khim. (Leningrad)*, 1968, **41**, 1544; *J. Appl. Chem. USSR (Engl. Transl.)*, 1968, **41**, 1470 (*ester*)
Dietze, U., *J. Prakt. Chem.*, 1974, **316**, 293 (*ir*)
Schulz, P.C., *An. Asoc. Quim. Argent.*, 1983, **71**, 271; *CA*, **100**, 15636 (*ir, Raman, cryst struct*)
Yuan, C. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1988, **37**, 205 (*dichloride, pmr*)
Maier, L., *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1990, **47**, 465 (*dichloride, synth, pmr*)

E

Eicosafluorononane, 9CI **E-1-00001**
Perfluorononane. Icosafluorononane
[375-96-2]

$F_3C(CF_2)_7CF_3$

C_9F_{20} M 488.0
d 1.80. Bp 125-126°. n_D^{20} 1.2760.
Musgrave, W.K.R. *et al*, *J.C.S.*, 1949, 3021 (*synth*)
Haszeldine, R.N. *et al*, *J.C.S.*, 1950, 3617 (*synth*)

1,20-Eicosanediol, 9CI **E-1-00002**
1,20-Icosanediol
[7735-43-5]

$HOCH_2(CH_2)_{18}CH_2OH$

$C_{20}H_{42}O_2$ M 314.5
Occurs in Carnauba wax and apple wax. Cryst. (C_6H_6 or EtOH). Mp 111-112° (103°). $Bp_{1.5}$ 215-217°.
Di-Ac:
$C_{24}H_{46}O_4$ M 398.6 Mp 64.5°.
Chuit, P. *et al*, *Helv. Chim. Acta*, 1929, **12**, 850 (*synth*)
Kimura, K. *et al*, *Chem. Pharm. Bull.*, 1960, **8**, 1059 (*di-Ac*)
Nakaya, T. *et al*, *Makromol. Chem.*, 1987, **188**, 265 (*synth*)
Percec, V. *et al*, *Macromolecules*, 1990, **23**, 3509 (*synth, pmr*)

10-Eicosene **E-1-00003**
10-Icosene
[66587-45-9]

$H_3C(CH_2)_8CH{=}CH(CH_2)_8CH_3$

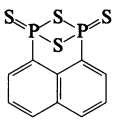
$C_{20}H_{40}$ M 280.5
Isol. from *Rosa damascena* (Bulgarian rose oil). Oil.
[78999-41-4, 78999-42-5]
Kovats, E., *J. Chromatogr.*, 1987, **406**, 185 (*isol*)
Collazo, L.R. *et al*, *J.O.C.*, 1993, **58**, 43 (*synth, ir, ms, pmr, cmr*)

4-Eicosenoic acid **E-1-00004**
4-Icosenoic acid

$H_3C(CH_2)_{14}CH{=}CHCH_2CH_2COOH$

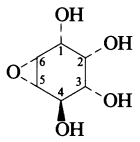
$C_{20}H_{38}O_2$ M 310.5
(Z)-form [82683-00-9]
(3-Hydroxy-11Z-eicosenyl) ester: [122576-62-9]. ***Drechslerol B***
$C_{40}H_{76}O_3$ M 605.0 Metab. of *Drechslera maydis*. Yellow viscous mass.
[82683-11-2]
Shukla, R.S. *et al*, *Phytochemistry*, 1989, **28**, 2089.

1,3-Epithio-1*H*,3*H*-naphtho[1,8-*c*,*d*][1,2,6]thiadiphosphorin 1,3-disulfide **E-1-00005**
Naphthalenedithiadiphosphetane disulfide
[115505-46-9]



$C_{10}H_6P_2S_4$ M 316.3
No phys. props. descr.
Wood, P.T. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1989, **41**, 51 (*synth, use, reaction, cryst struct*)

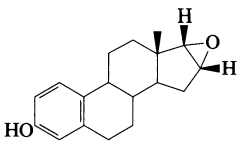
5,6-Epoxy-1,2,3,4-cyclohexanetetrol **E-1-00006**
1,2-Anhydroinositol, 9CI. 7-Oxabicyclo[4.1.0]heptane-1,2,3,4-tetrol



(1α,2α,3α,4β,5α,6α)-*form*

$C_6H_{10}O_5$ M 162.1
(1α,2α,3α,4β,5α,6α)-form [80736-38-5]
1,2-Anhydro-epi-*inositol, 9CI. Conduritol C* cis-*epoxide*
Specific β-glycosidase inhibitor. Cryst. Mp 126° (110-127°). Racemate.
Tetra-Ac:
$C_{14}H_{18}O_9$ M 330.2 Prisms (EtOH). Mp 115.5-116.5°.
(1α,2α,3α,4β,5β,6β)-form [80736-37-4]
1,2-Anhydro-neo-*inositol, 9CI. Conduritol C* trans-*epoxide*
α-Galactosidase inhibitor. Cryst. (EtOH). Mp 145° (130-143°). Racemate.
Tetra-Ac: Cryst. ($EtOH/H_2O$). Mp 114-115°.
(1α,2α,3β,4β,5α,6α)-form [23559-36-6]
1,2-Anhydro-allo-*inositol, 9CI. Conduritol E epoxide*
Mp 176-177°. Racemate. Known also in opt. active form (+)-form +153 (c, 0.5 in H_2O).
Tetranitrate: [23627-80-7].
$C_6H_6N_4O_{13}$ M 342.1 Cryst. (EtOH). Mp 89-89.2°.
(1α,2β,3α,4β,5α,6α)-form [6090-95-5]
1,2-Anhydro-DL-myo-*inositol, 9CI. Conduritol B epoxide*
Inhibitor of the enzyme which cleaves glucosylceramide. The enzyme is defective in the human genetic disorder Gaucher disease. Cryst. (EtOH). Mp 155-156°. Racemate.
Angyal, S.J. *et al*, *J.C.S.*, 1957, 3691 ((+)-*Conduritol E epoxide*)
Nakajima, M. *et al*, *Chem. Ber.*, 1959, **92**, 173; 1961, **94**, 515 (*synth, ir*)
Legler, G., *Z. Physiol. Chem.*, 1966, **345**, 197 (*synth*)
Anikeeva, A.N. *et al*, *Zh. Obshch. Khim.*, 1966, **36**, 194; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1966, **36**, 203 (*ir*)
Eremenko, L.T. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1970, 920; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1970, 920 (*Conduritol E tetranitrates*)
Legler, G. *et al*, *FEBS Lett.*, 1981, **135**, 139 (*synth, biochem*)
Lee, K.J. *et al*, *Carbohydr. Res.*, 1985, **144**, 148 (*synth, Conduritol B epoxide*)
Gal, A.E. *et al*, *J. Labelled Compd. Radiopharm.*, 1987, **24**, 397; *CA*, **108**, 55775k (*synth*)
Datta, S.C. *et al*, *Biochem. Biophys. Res. Commun.*, 1988, **152**, 155 (*biochem*)
Carless, H.A.J., *Tet. Lett.*, 1992, **33**, 6379 (*synth, pmr, cmr, Conduritol E epoxides*)

16,17-Epoxyestra-1,3,5(10)-trien-3-ol, 9CI **E-1-00007**



(16α,17α)-*form*

$C_{18}H_{22}O_2$ M 270.3
(16α,17α)-form [472-56-0] ***Estroxide***
Metab. of estratetraenol.
(16β,17β)-form [472-57-1]
Needles (C_6H_6/petrol). Mp 194-197°. $[\alpha]_D^{25}$ +119 ($CHCl_3$).
Ac:
$C_{20}H_{24}O_3$ M 312.4 Cryst. (petrol). Mp 117-118°. $[\alpha]_D^{27}$ +103.
Fishman, J. *et al*, *J.O.C.*, 1958, **23**, 1190 (*synth*)
Fishman, J., *J.A.C.S.*, 1960, **82**, 6143 (*Ac*)
Watabe, T. *et al*, *J. Biol. Chem.*, 1979, **254**, 10720 (*formn*)
Siekmann, L. *et al*, *Acta Endocrinol. (Copenhagen)*, 1980, **95**, 49 (*biosynth*)
Arunachalam, T. *et al*, *J.O.C.*, 1981, **46**, 3415 (*synth, pmr*)

1,1,1-Ethanetricarbonitrile, 9CI **E-1-00008**
1,1,1-Tricyanoethane. Methylcyanoform
[10359-20-3]

$H_3CC(CN)_3$

$C_5H_3N_3$ M 105.0
Cryst. (CH_2Cl_2); needles by subl. Mp 94°.
Hantzch, A. *et al*, *Ber.*, 1899, **32**, 641 (*synth*)
Witt, J.R. *et al*, *Acta Cryst. B*, 1972, **28**, 950 (*cryst struct*)
Gattow, G. *et al*, *Z. Anorg. Allg. Chem.*, 1992, **611**, 134 (*synth, ir, Raman, cmr, ms*)
Rüchardt, C. *et al*, *Chem. Ber.*, 1994, **127**, 2225 (*synth*)

1,1,1-Ethanetricarboxylic acid **E-1-00009**

$H_3CC(COOH)_3$

$C_5H_6O_6$ M 162.0
Unknown in the free state.

Tri-Me ester: [5537-85-9].
$C_8H_{12}O_6$ M 204.1 Prisms (petrol or MeOH). Mp 39°. Bp_{15} 123-124°.

Et, Di-Me ester: [74896-32-5].
$C_9H_{14}O_6$ M 218.2 Bp_2 93°.

Tri-Et ester: [16515-90-5].
$C_{11}H_{18}O_6$ M 246.2 Bp_{10} 130-132°.

Trinitrile: see *1,1,1-Ethanetricarbonitrile, E-1-00008*

Arndt, F. *et al, Annalen*, 1932, **499**, 228 (*tri-Me ester*)
Prelicz, D. *et al, Pol. J. Chem.* (*Rocz. Chem.*), 1967, **41**, 267 (*tri-Et ester*)
Saitkulova, F.G. *et al, Zh. Prikl. Khim.* (*Leningrad*), 1981, **54**, 206; *CA*, **94**, 208317g (*esters*)

1,2-Ethenediylbisphosphonic acid, 9CI E-1-00010

$(HO)_2P(O)CH{=}CHP(O)(OH)_2$

$C_2H_6O_6P_2$ M 188.0

(E)-form [34169-22-7]
Cryst. + $1H_2O$. Mp 194.5-196°. Dehyrated at 240°. Dec. 400°.

Tetra-Me ester: [25362-05-4]. *Tetramethyl 1,2-ethenediylbisphosphonate*
$C_6H_{14}O_6P_2$ M 244.1 Solid or liq. Mp 29-30°. $Bp_{0.9}$ 135-140°.

Tetra-Et ester: [20408-22-4]. *Tetraethyl 1,2-ethenediylbisphosphonate*
$C_{10}H_{22}O_6P_2$ M 300.2 Liq. $Bp_{0.05}$ 140-143°. n_D^{23} 1.4491.

Tetrachloride:
$C_2H_2Cl_4O_2P_2$ M 261.7 Solid. Mp 154-156°.

Tavs, P. *et al, Tetrahedron*, 1970, **26**, 5329 (*ester, synth, ir*)
Maier, L., *Phosphorus Relat. Group V Elem.*, 1973, **3**, 19 (*synth, derivs*)
Kruglov, S.V. *et al, Zh. Obshch. Khim.*, 1973, **43**, 1480; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1973, **43**, 1470 (*esters, synth, pmr*)
Pudovik, A.N. *et al, Zh. Obshch. Khim.*, 1973, **43**, 1647; 1976, **46**, 2492; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1973, **43**, 1629; 1976, **46**, 2385 (*synth*)
Samitov, Y.Y. *et al, Zh. Obshch. Khim.*, 1975, **45**, 2130; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1975, **45**, 2097 (*esters, synth, pmr, P-31 nmr*)
Klose, G. *et al, Chem. Phys. Lett.*, 1990, **175**, 472 (*tetraethyl ester, P-31 nmr*)
Harris, R.K. *et al, Magn. Reson. Chem.*, 1993, **31**, 1085 (*esters, cmr, P-31 nmr*)

(2-Ethoxyethenyl)phosphonous acid E-1-00011

(2-Ethoxyvinyl)phosphonous acid

$EtOCH{=}CHP(OH)_2$

$C_4H_9O_3P$ M 136.0
cis and *trans*-forms of esters have been characterised spectroscopically.

Di-Me ester: [37916-74-8]. *Dimethyl (2-ethoxyethenyl)phosphonite*
$C_6H_{13}O_3P$ M 164.1 Liq. d_4^{20} 1.03. $Bp_{15.5}$ 81-82°. n_D^{20} 1.4618.

Di-Et ester: [37916-75-9]. *Diethyl (2-ethoxyethenyl)phosphonite*
$C_8H_{17}O_3P$ M 192.1 d_4^{20} 0.98. $Bp_{11.5}$ 93°. n_D^{20} 1.4567.

Dipropyl ester: [62170-64-3]. *Dipropyl (2-ethoxyethenyl)phosphonite*
$C_{10}H_{21}O_3P$ M 220.2 Liq. d_4^{20} 0.96. Bp_3 95-97°. n_D^{20} 1.4487.

Diisopropyl ester: [62170-63-2]. *Diisopropyl (2-ethoxyethenyl)phosphonite*
$C_{10}H_{21}O_3P$ M 220.2 Liq. d_4^{20} 0.96. Bp_3 88-90°. n_D^{20} 1.4469.

Bis(2,2,3,3-tetrafluoropropyl)ester: [62170-66-5]. *Bis(2,2,3,3-tetrafluoropropyl) (2-ethoxyethenyl)phosphonite*
$C_{10}H_{13}F_8O_3P$ M 364.1 Liq. d_4^{20} 1.43. Bp_2 138-140°. n_D^{20} 1.4130.

Dibutyl ester: [62170-65-4]. *Dibutyl (2-ethoxyethenyl)phosphonite*
$C_{12}H_{25}O_3P$ M 248.3 Liq. d_4^{20} 0.93. Bp_4 118-120°. n_D^{20} 1.4429.

[69246-22-6, 69246-23-7, 69246-24-8, 69246-25-9, 75554-31-3, 75554-32-4, 75554-33-5, 75554-34-6]

Foss, V.L. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1962, **146**, 1106.
Anisimov, K.N. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1962, 442.
Krylov, L.V. *et al, Zh. Obshch. Khim.*, 1976, **46**, 2513; 1978, **48**, 2473; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1976, **46**, 2403; 1978, **48**, 2245 (*synth, pmr, P-31 nmr*)

1-Ethoxy-1-octyne, 9CI E-1-00012

Ethyl 1-octynyl ether, 8CI

[14273-09-7]

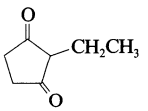
$H_3C(CH_2)_5C{\equiv}COEt$

$C_{10}H_{18}O$ M 154.2
Oil. $Bp_{9.5}$ 80-81°, $Bp_{0.2}$ 30°.

McCarney, C.C. *et al, Tetrahedron*, 1976, **32**, 1189 (*synth, pmr*)
Pons, J.-M. *et al, Tet. Lett.*, 1989, **30**, 1833 (*synth*)
Pons, J.-M. *et al, Synthesis*, 1994, 1294 (*synth*)

2-Ethyl-1,3-cyclopentanedione, 9CI E-1-00013

[823-36-9]



$C_7H_{10}O_2$ M 126.1
Precursor for the D-ring in the total synth. of steroids. Cryst. (H_2O). Mp 175-177°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 253A.
Schick, H. *et al, Chem. Ber.*, 1969, **102**, 3238 (*synth*)
Martinez, R.A. *et al, Synth. Commun.*, 1989, **19**, 373 (*synth, pmr*)

4-Ethylcyclopentene E-1-00014

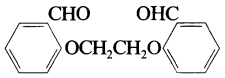
C_7H_{12} M 96.1
d^{20} 0.798. Bp 106°. n_D^{20} 1.4400.

Adv. Chem. Ser., 1955, **15**, 421 (***props***)

2,2′-Ethylenedioxybisbenzaldehyde E-1-00015

2,2′-[1,2-Ethanediylbis(oxy)]bisbenzaldehyde, 9CI. 1,4-Bis(2-formylphenyl)-1,4-dioxabutane

[52118-10-2]



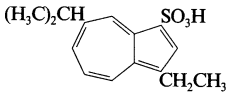
$C_{16}H_{14}O_4$ M 270.2
Useful starting material for crown ethers and macrocyclic ligands. Needles. Mp 129°.

Armstrong, L.G. *et al, Inorg. Chem.*, 1975, **14**, 1322 (*synth*)
Atkinson, I.M. *et al, Aust. J. Chem.*, 1994, **47**, 1155 (*use*)

3-Ethyl-7-isopropyl-1-azulenesulfonic acid E-1-00016

3-Ethyl-7-(1-methylethyl)-1-azulenesulfonic acid. ***Egualen, INN.*** *Azuletil. KT 1-32*

[99287-30-6]



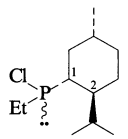
$C_{15}H_{18}O_3S$ M 278.3
Thromboxane A_2-receptor antagonist. Antiulcer agent.

Na salt: [97683-31-3].
Bluish-violet cryst. Mp 152-154° dec.
▶ LD_{50} (rat, orl) 1096 mg/kg. LD_{50} (rat, ipr) 224 mg/kg. CO4825000.

Eur. Pat., 147 915, (1985) (*Kotobuki Seiyaku*); *CA*, **104**, 68494k (*synth, pharmacol*)
Yanagisawa, T. *et al, Chem. Pharm. Bull.*, 1988, **36**, 641; 1991, **39**, 2429 (*synth, ir, pmr, pharmacol*)
Mochizuki, S. *et al, Scand. J. Gastroenterol., Suppl.*, 1989, **162**, 194 (*pharmacol*)

Ethyl(2-isopropyl-5-methylcyclohexyl) phosphinous chloride, 8CI E-1-00017

Ethyl[5-methyl-2-(1-methylethyl)cyclohexyl] phosphinous chloride, 9CI. Chloroethyl(2-isopropyl-5-methylcyclohexyl)phosphine

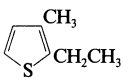


$C_{12}H_{24}ClP$ M 234.7
(1R,2S,5R)-form
Ethylmenthylphosphinous chloride. Chloroethylmenthylphosphine
Liq. $Bp_{0.2}$ 95°. Diastereoisomers epimeric at P recognised spectroscopically.

[113613-07-3, 113613-09-5]

Hägele, G. *et al, J.C.S. Dalton*, 1987, 795 (*synth, pmr, cmr, P-31 nmr*)

2-Ethyl-3-methylthiophene E-1-00018



$C_7H_{10}S$ M 126.2
d^{20} 0.982. Bp 161°. n_D^{20} 1.5105.

[86701-25-9]

Adv. Chem. Ser., 1955, **15**, 196 (***props***)

3-Ethyl-2-methylthiophene, 9CI E-1-00019

[53119-51-0]

$C_7H_{10}S$ M 126.2
Bp 157°.

Adv. Chem. Ser., 1955, **15**, 197 (***props***)

3-Ethyl-2,4-pentanedione, 9CI E-1-00020

Ethylacetylacetone. 3-Ethyl-4-hydroxy-3-penten-2-one

[1540-34-7]

$H_3CCH_2CH(COCH_3)_2 \rightleftharpoons H_3CCH_2C(COCH_3)=C(CH_3)OH$

$C_7H_{12}O_2$ M 128.1
About 25% enol form in pure liq., over 40% enol in some solvs. (CCl_4, C_6H_6). d_4^{20} 0.9568. Bp 179°, Bp_{20} 76°. n_D^{20} 1.4419.

[34135-99-4]

v. Auwers, K. *et al*, *Annalen*, 1921, **426**, 161, 227 (*synth*)
Morgan, G.T. *et al*, *J. Soc. Chem. Ind., London*, 1925, **44**, 462 (*synth*)
Johnson, A.W. *et al*, *J.C.S.*, 1958, 4254 (*synth*)
Yoffe, S.T. *et al*, *Tetrahedron*, 1962, **18**, 923 (*tautom, ir, uv*)
Ioffe, S.T. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1965, 1556; 1968, 2024; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1965, 1523; 1968, 1927 (*tautom, pmr*)
Emsley, J. *et al*, *J. Mol. Struct.*, 1987, **161**, 193 (*synth, tautom*)
McLendon, G. *et al*, *J.A.C.S.*, 1992, **114**, 6227 (*synth, pmr*)
Nölke, M. *et al*, *Annalen*, 1995, 41 (*synth, pmr*)

3-Ethylpentanoic acid E-1-00021

3,3-Diethylpropanoic acid

[58888-87-2]

$(H_3CCH_2)_2CHCH_2COOH$

$C_7H_{14}O_2$ M 130.1
Me ester: [63540-23-8].
$C_8H_{16}O_2$ M 144.2 Bp 164°.
Amide: [55327-21-4].
$C_7H_{15}NO$ M 129.2 Cryst. (EtOH). Mp 130°.
Nitrile: [5631-83-4].
$C_7H_{13}N$ M 111.1 Bp_{12} 60°.

Doering, W. von E. *et al*, *J.A.C.S.*, 1956, **78**, 4947 (*ester*)
Cohen-Addad, C. *et al*, *Acta Cryst. B*, 1975, **31**, 835 (*synth, cryst struct, amide*)
Degenhardt, C.R., *Synth. Commun.*, 1982, **12**, 415 (*synth*)

Ethyl phenyl disulfide, 9CI E-1-00022

[4032-81-9]

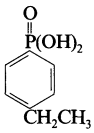
Ph—S—S—Et

$C_8H_{10}S_2$ M 170.2
Liq. Bp_{14} 123°, $Bp_{0.7}$ 94°. n_D^{25} 1.5980.

Lecher, H. *et al*, *Ber.*, 1922, **55**, 1474 (*synth*)
Armitage, D.A. *et al*, *J.C.S. Perkin 1*, 1972, 680 (*synth*)
Capozzi, G. *et al*, *Gazz. Chim. Ital.*, 1990, **120**, 421 (*synth, pmr, ms*)

(4-Ethylphenyl)phosphonic acid E-1-00023

[6873-66-1]



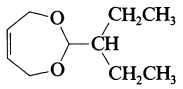
$C_8H_{11}O_3P$ M 186.1
Di-Et ester: [72596-29-3]. *Diethyl (4-ethylphenyl)phosphonate*
$C_{12}H_{19}O_3P$ M 242.2 Liq. $Bp_{0.9}$ 132-134°.
Monohexyl ester: [128333-47-1]. *Monohexyl (4-ethylphenyl)phosphonate*
$C_{14}H_{23}O_3P$ M 270.3 pK_a 3.55.
Dichloride: [74289-32-0].
$C_8H_9Cl_2OP$ M 223.0 Liq. d^{20} 1.29. $Bp_{1.5}$ 100-100.5°. n_D^{20} 1.5521.

Kabachnik, M.I. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1961, 1896; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1961, 1770 (*dichloride*)
Dietze, U., *J. Prakt. Chem.*, 1974, **316**, 485 (*ir*)
Morita, T. *et al*, *Chem. Lett.*, 1980, 435 (*dichloride*)
Yuan, C. *et al*, *Synthesis*, 1990, 140 (*esters, synth, P-31 nmr*)
Hu, W. *et al*, *Chin. Chem. Lett.*, 1992, **3**, 579 (*P-31 nmr*)
Yuan, C. *et al*, *Heteroat. Chem.*, 1993, **4**, 23 (*P-31 nmr*)

2-(1-Ethylpropyl)-4,7-dihydro-1,3-dioxepin, 9CI E-1-00024

4,7-Dihydro-2-(3-pentyl)-1,3-dioxepin. Karotine

[53338-06-0]



$C_{10}H_{18}O_2$ M 170.2
Perfumery ingredient. Liq. d 0.95.

Ger. Pat., 2 407 863, (1974); *CA*, **82**, 4332a.

(1-Ethylpropylidene) propanedioic acid, 9CI E-1-00025

(1-Ethylpropylidene)malonic acid. 2-Ethyl-1-butene-1,1-dicarboxylic acid

$(H_3CCH_2)_2C=C(COOH)_2$

$C_8H_{12}O_4$ M 172.1
Di-Et ester: [78775-59-4].
$C_{12}H_{20}O_4$ M 228.2 Liq. $Bp_{0.3}$ 80°.
Mononitrile: [868-01-9]. *2-Cyano-3-ethyl-2-pentenoic acid, 9CI*
$C_8H_{11}NO_2$ M 153.1 No phys. props. reported.
Mononitrile, Me ester: [22863-91-8].
$C_9H_{13}NO_2$ M 167.2 Bp_5 105-106°.
Mononitrile, Et ester: [868-04-2].
$C_{10}H_{15}NO_2$ M 181.2 Bp_{11} 118°.
Dinitrile: [10394-95-3]. *3-(Dicyanomethylene) pentene*
$C_8H_{10}N_2$ M 134.1 Liq. Bp_{23} 120-123°.

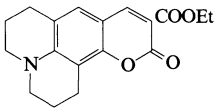
[142438-74-2]

Cope, A.C. *et al*, *J.A.C.S.*, 1937, **59**, 2327; 1941, **63**, 733 (*nitriles*)
Hamelin, J. *et al*, *Bull. Soc. Chim. Fr.*, 1968, 2513 (*deriv*)
Wisfield, D.G. *et al*, *Can. J. Chem.*, 1970, **48**, 855 (*dinitrile*)
Holmberg, C. *et al*, *Annalen*, 1981, 748 (*Et ester*)
Texier-Boullet, F. *et al*, *Tet. Lett.*, 1982, **23**, 4927 (*dinitrile*)

Ethyl 2,3,6,7-tetrahydro-11-oxo-1*H*,5*H*,11*H*-[1]benzopyrano[6,7,8-*ij*]quinolizine-10-carboxylate, 9CI E-1-00026

Coumarin 314

[55804-66-5]

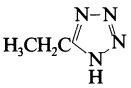


$C_{18}H_{19}NO_4$ M 313.3
Laser dye. Mp 140-144°. λ_{max} 436 nm.

Yip, B.C. *et al*, *Acta Cryst. C*, 1995, **51**, 956 (*cryst struct, bibl*)

5-Ethyl-1*H*-tetrazole, 9CI E-1-00027

[16687-59-5]

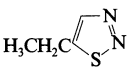


$C_3H_6N_4$ M 98.1
Cryst. (EtOAc). Mp 98-99°.

Mihina, J.S. *et al*, *J.O.C.*, 1950, **15**, 1082 (*synth*)

5-Ethyl-1,2,3-thiadiazole E-1-00028

[50406-55-8]



$C_4H_6N_2S$ M 114.1
$Bp_{0.3}$ 46°.

Heier, H. *et al*, *Annalen*, 1986, 1334 (*synth, ir, pmr, cmr, ms*)
L'abbé, G. *et al*, *J. Het. Chem.*, 1993, **30**, 301 (*N-15 nmr*)

2-(Ethylthio)-1,3-butadiene E-1-00029

[7326-63-8]

$C_6H_{10}S$ M 114.2
Diels-Alder diene.

Negishi, E. *et al*, *J.O.C.*, 1983, **48**, 1562 (*synth, ir, pmr, cmr*)
Trofimov, B.A. *et al*, *Sulfur Lett.*, 1986, **4**, 125.
Narasaka, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1991, **64**, 387.

1-(Ethylthio)-1-buten-3-yne E-1-00030

HC≡CCH=CHSEt

C_6H_8S M 112.1
(***Z*)-*form*** [19458-01-6]
Yellow liq. Bp_{12} 64°. n_D^{20} 1.5440.

Volkov, A. *et al*, *Zh. Org. Khim.*, 1982, **18**, 269 (*synth*)
Fossatelli, M. *et al*, *Tet. Lett.*, 1992, **33**, 4229 (*synth*)

Ethylvinylphosphinic acid E-1-00031

Ethenylethylphosphinic acid

$H_2C{=}CHPEt(O)OH$

$C_4H_9O_2P$ M 120.0

Me ester: [56542-09-7]. *Methyl ethylvinylphosphinate*
$C_5H_{11}O_2P$ M 134.1 Liq. d_4^{20} 1.05. Bp_{11} 80°. n_D^{20} 1.4518.

Et ester: [10545-62-7]. *Ethyl ethylvinylphosphinate*
$C_6H_{13}O_2P$ M 148.1 Liq. d_4^{20} 1.02. Bp_{14} 86.5°. n_D^{20} 1.4495.

2-Propenyl ester: 2-Propenyl ethenylethylphosphinate. Allyl ethylvinylphosphinate
$C_7H_{13}O_2P$ M 160.1 d_4^{20} 1.02. Bp_{10} 99-100°. n_D^{20} 1.4640.

Propyl ester: [71431-36-2]. *Propyl ethylvinylphosphinate*
$C_7H_{15}O_2P$ M 162.1 Liq. d_4^{20} 0.99. Bp_{10} 94-95°. n_D^{20} 1.4468.

Isopropyl ester: [88093-32-7]. *Isopropyl ethylvinylphosphinate*
$C_7H_{15}O_2P$ M 162.1 Liq. d_4^{20} 0.98. Bp_{10} 83°. n_D^{20} 1.4440.

Ph ester: Phenyl ethylvinylphosphinate
$C_{10}H_{13}O_2P$ M 196.1 Liq. d_4^{20} 1.11. Bp_3 114-115°. n_D^{20} 1.5240.

Diethylamide: [56542-10-0]. P-*Ethenyl*-N,N,P-*triethylphosphinic amide*
$C_8H_{18}NOP$ M 175.2 Liq. d_4^{20} 1.0. $Bp_{0.035}$ 52-53°. n_D^{20} 1.4745.

Kamai, G. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1959, **128**, 543; *CA*, **54**, 7538.
Tsivunin, V.S. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1960, **131**, 1113; *CA*, **54**, 20843.
Pyrkin, R.I. *et al*, *Zh. Obshch. Khim.*, 1975, **45**, 762; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1975, **45**, 750 (*Me ester, amide, synth, P-31 nmr*)

1,2-Ethynediylbisphosphonic acid E-1-00032

Bis(dihydroxyphosphinyl)ethyne. Diphosphonoacetylene

[41391-90-6]

$(HO)_2P(O)C{\equiv}CP(O)(OH)_2$

$C_2H_4O_6P_2$ M 185.9
Ester undergoes Diels-Alder reactions giving cycloalkenebisphosphonic esters and leading to aromatic 1,2-diphosphonic acids. Viscous dihydrate.

Bis(tributylammonium) salt: [92340-87-9]. Hygroscopic powder + $1H_2O$. Mp 130-135°.

Tetra-Me ester: [19519-58-5]. *Tetramethyl 1,2-ethynediylbisphosphonate*
$C_6H_{12}O_6P_2$ M 242.1 Solid or liq. Mp 13-15°. Bp_{15} 155-156°. n_D^{25} 1.4476.

P,P-*Di-Me*, P′,P′-*di-Et ester:* P,P-*Dimethyl*, P′,P′-*diethyl 1,2-ethynediylbisphosphonate*
$C_8H_{16}O_6P_2$ M 270.1 Liq. d_4^{20} 1.20. Bp_1 151-153°. n_D^{20} 1.4495.

Tetra-Et ester: [4851-53-0]. *Tetraethyl 1,2-ethynediylbisphosphonate*
$C_{10}H_{20}O_6P_2$ M 298.2 Liq. d_4^{20} 1.12. $Bp_{2.5}$ 181.5-182.5°. n_D^{20} 1.4475.

Tetraisopropyl ester: Tetrakis(1-methylethyl) 1,2-ethynediylbisphosphonate
$C_{14}H_{28}O_6P_2$ M 354.3 Liq. $Bp_{0.1}$ 140°. n_D^{20} 1.4435.

Ionin, B.I. *et al*, *Zh. Obshch. Khim.*, 1965, **35**, 1917; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1965, **35**, 1910 (*Tetra-Et ester*)
Seyferth, D. *et al*, *J.O.C.*, 1969, **34**, 1483 (*Tetra-Me ester*)
Maier, L., *Phosphorus Relat. Group V Elem.*, 1973, **2**, 229 (*synth, esters, pmr, P-31 nmr*)
Kruglov, S.V. *et al*, *Zh. Obshch. Khim.*, 1973, **43**, 1480; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1973, **43**, 1470.
Blackburn, G.M. *et al*, *J.C.S. Perkin 1*, 1984, 1119; 1991, 286 (*synth, ms, pmr, P-31 nmr*)
Ziegler, T. *et al*, *Chem. Ber.*, 1987, **120**, 1347 (*use*)

1,2-Ethynediylbis [triphenylbis(phenylethynyl) phosphorane], 9CI E-1-00033

[147437-85-2]

$PhC{\equiv}CPPh_3C{\equiv}CPPh_3C{\equiv}CPh$

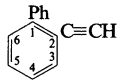
$C_{54}H_{40}P_2$ M 750.8
Brown cryst. Mp 43-58° dec. With H_2O → Ph_3PO + $PhC{\equiv}CH$. When heated → Ph_3P + Ph_3PO.

Ogawa, S. *et al*, *Tet. Lett.*, 1993, **34**, 838 (*synth, ms, pmr, cmr, P-31 nmr, props*)

2-Ethynyl-1,1′-biphenyl, 9CI E-1-00034

2-Biphenylylacetylene

[52889-62-0]



$C_{14}H_{10}$ M 178.2
Oil. Bp_3 137°.

Faseeh, S.A. *et al*, *Indian J. Chem.*, 1947, **24**, 57 (*synth*)
Nourmamode, A. *et al*, *Bull. Soc. Chim. Fr.*, Part II, 1981, 207 (*synth, pmr, ir*)
Stephens, E.B. *et al*, *Macromolecules*, 1993, **26**, 2420 (*synth, ir, pmr*)

3-Ethynyl-1,1′-biphenyl, 9CI E-1-00035

3-Biphenylylacetylene

[58650-11-6]

$C_{14}H_{10}$ M 178.2
Liq. $Bp_{0.4}$ 98-100°. n_D^{25} 1.6300.

U.S. Pat., 3 968 251, (1976); *CA*, **85**, 116915m (*synth*)
Hofmann, J. *et al*, *Annalen*, 1995, 631 (*ir, ms*)

4-Ethynyl-1,1′-biphenyl, 9CI E-1-00036

4-Biphenylylacetylene

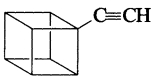
[29079-00-3]

$C_{14}H_{10}$ M 178.2
Cryst. (EtOH, CCl_4 or hexane/$CHCl_3$). Mp 86-87°.

Jacobs, T.L. *et al*, *J.O.C.*, 1957, **22**, 1424 (*synth*)
Tani, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1963, **36**, 391 (*synth, ir, uv*)
Dawson, D.A. *et al*, *Can. J. Chem.*, 1975, **53**, 373 (*cmr*)
Uno, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1992, **65**, 210 (*ir, pmr, ms*)
Stephens, E.B. *et al*, *Macromolecules*, 1993, **26**, 2420 (*synth, ir, pmr*)
Hofmann, J. *et al*, *Annalen*, 1995, 631 (*ir, ms*)
Yashima, E. *et al*, *Macromolecules*, 1995, **28**, 4184 (*synth, pmr*)

Ethynylcubane E-1-00037

Cubylacetylene



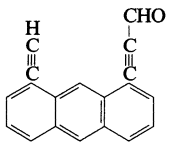
$C_{10}H_8$ M 128.1
Cryst. Mp 43-45°.

Eaton, P.E. *et al*, *J.A.C.S.*, 1994, **116**, 7588 (*synth, pmr, cmr*)

8-Ethynyl-1-(2-formylethynyl) anthracene E-1-00038

3-(8-Ethynyl-1-anthracenyl)-2-propynal

[157993-37-8]

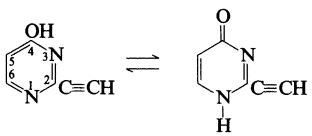


$C_{19}H_{10}O$ M 254.2
Yellow powder. Mp 130-131°.

Breitmaier, E. *et al*, *Annalen*, 1994, 857 (*synth, pmr, cmr, ms*)

2-Ethynyl-4-hydroxypyrimidine E-1-00039

2-Ethynyl-4(1H)-pyrimidinone. 2-Ethynyl-4-pyrimidinol



OH-form *NH-form*

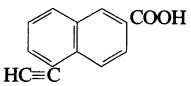
$C_6H_4N_2O$ M 120.1

OH-form

Me ether: [161489-04-9]. *2-Ethynyl-4-methoxypyrimidine, 9CI*
$C_7H_6N_2O$ M 134.1 Solid by subl. Mp 88.0-89.5°. $Subl._{0.5}$ 50°.

Boucher, E. *et al*, *J.O.C.*, 1995, **60**, 1408 (*Me ether, synth, ir, pmr, cmr*)

5-Ethynyl-2-naphthalenecarboxylic acid E-1-00040



$C_{13}H_8O_2$ M 196.2
Solid. Mp 247-248°.

Ellingboe, J.W. *et al*, *J. Med. Chem.*, 1993, **36**, 2485 (*synth, pmr*)

1-Ethynyl-1*H*-pyrrole, 9CI E-1-00041

[139565-93-8]

C_6H_5N M 91.1
Liq. Bp 108°. n_D^{20} 1.513. Turns brown at r.t.

Paley, M.S. *et al*, *J.A.C.S.*, 1992, **114**, 3247 (*synth, pmr*)
Brandsma, L. *et al*, *Synth. Commun.*, 1994, **24**, 2721 (*synth*)

2-Ethynyl-1*H*-pyrrole, 9CI E-1-00042

[67237-51-8]

C_6H_5N M 91.1
Nitrification inhibitor. Liq. $Bp_{0.01}$ 40°. Polymerises at r.t.

N-*Me:* [67237-52-9].
C_7H_7N M 105.1 Liq. Bp 147-148°, Bp_{10} 52-53°.

Wentrup, C. *et al*, *Angew. Chem.*, 1978, **90**, 643 (*synth, pmr, ir*)
Maquestiau, A. *et al*, *Org. Mass Spectrom.*, 1978, **13**, 518 (*ms*)

3-Ethynyl-1*H*-pyrrole E-1-00043

[71580-43-3]

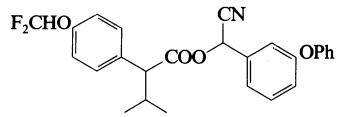
C_6H_5N M 91.1
Unstable oil.

N-*Me:* [66463-25-0].
C_7H_7N M 105.1 Mp 29-30°.

Shil'nikova, L.N. *et al*, *Zh. Org. Khim.*, 1978, **14**, 251; *J. Org. Chem. USSR* (*Engl. Transl.*), 1978, **14**, 232 (*N-Me*)
Muchowski, J.M. *et al*, *J.O.C.*, 1992, **57**, 1653 (*synth*)

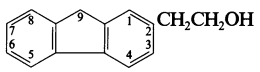
F

Flucythrinate, BSI, ANSI, ISO F-1-00001
Cyano(3-phenoxyphenyl)methyl 4-(difluoromethoxy)-α-(1-methylethyl) benzeneacetate, 9CI. α-Cyano-3-phenoxybenzyl 2-(4-difluoromethoxyphenyl)-3-methylbutyrate. Cybolt. Cythrin
[70124-77-5]



$C_{26}H_{23}F_2NO_4$ M 451.4
Pyrethroid insecticide. Various stereoisomers prepd.
▶ LD_{50} (rat, orl) 81 mg/kg.
[77104-40-6, 80845-23-4, 80845-25-6, 81601-15-2, 81601-16-3, 81601-17-4]
U.S. Pat., 4 307 036, (1981); *CA*, **96**, 199337a (*synth, activity*)
Horiba, M. *et al, Agric. Biol. Chem.*, 1982, **46**, 3041 (*abs config, cd, uv*)
Chapman, R.A., *J. Chromatogr.*, 1983, **258**, 175 (*hplc*)
Wettstein, K., *Meded. Fac. Landbouwwet., Rijksuniv. Gent*, 1983, **48**, 331 (*rev*)
Pesticide Manual, 9th edn., 1991, No. 6440.

9*H*-Fluorene-2-ethanol, 9CI F-1-00002
2-(2-Hydroxyethyl)fluorene. 2-(2-Fluorenyl) ethanol
[87776-79-2]

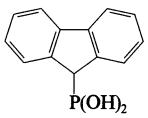


$C_{15}H_{14}O$ M 210.2
Leaflets (petrol). Mp 136-137° (132.5-134.5°).
Ac:
$C_{17}H_{16}O_2$ M 252.3 Leaflets (petrol). Mp 94-95°.
Profft, E. *et al, J. Prakt. Chem.*, 1963, **22**, 47 (*synth, ir*)
Tsuno, Y. *et al, CA*, 1983, **99**, 194102x (*synth*)

9*H*-Fluorene-4-ethanol F-1-00003
4-(2-Hydroxyethyl)fluorene. 2-(4-Fluorenyl) ethanol
$C_{15}H_{14}O$ M 210.2
Clusters (petrol). Mp 81-82°.
Ac:
$C_{17}H_{16}O_2$ M 252.3 Mp 52-53°.
Profft, E. *et al, J. Prakt. Chem.*, 1963, **22**, 47 (*synth, ir*)

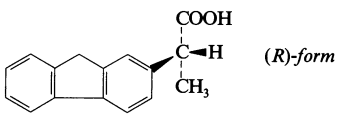
9*H*-Fluorene-9-ethanol, 9CI F-1-00004
9-(2-Hydroxyethyl)fluorene. 2-(9-Fluorenyl) ethanol
[3952-36-1]
$C_{15}H_{14}O$ M 210.2
Needles (C_6H_6 or toluene/hexane). Mp 107-108° (98-99°).
Me ether: [57722-05-1]. *9-(2-Methoxyethyl)-9H-fluorene, 9CI*
$C_{16}H_{16}O$ M 224.3 $Bp_{0.5}$ 143°.
Greenhow, E.J. *et al, J.C.S.*, 1951, 2848 (*synth*)
Jones, D.W. *et al, J.C.S.(B)*, 1971, 389 (*pmr*)
Maercker, A. *et al, Chem. Ber.*, 1983, **116**, 710 (*synth, pmr*)
Rieger, B. *et al, Organometallics*, 1994, **13**, 647 (*synth, pmr*)
Perumattam, J. *et al, Synthesis*, 1994, 1181 (*synth, ir, pmr*)

9*H*-Fluoren-9-ylphosphonous acid F-1-00005
9-Fluorenephosphonous acid



$C_{13}H_{11}O_2P$ M 230.2
Di-Et ester: Diethyl 9H-9-fluorenylphosphonite
$C_{17}H_{19}O_2P$ M 286.3 Solid. Mp 67.5-70°. Bp_2 148.5-149°.
Bis(diethylamide): [148115-62-2]. N,N,N′,N′-*Tetraethyl*-P-9H-*fluoren-9-ylphosphonous diamide*
$C_{21}H_{29}N_2P$ M 340.4 Solid. Mp 84-86°.
Bis(diisopropylamide): [148115-63-3]. P-9H-*Fluoren-9-yl*-N,N,N′,N′-*tetrakis(1-methylethyl)phosphonous diamide*
$C_{25}H_{37}N_2P$ M 396.5 Solid. Mp 132-134°.
Kabachnik, M.I. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1960, 133; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1960, 122.
Kolodyazhnyi, O.I. *et al, Zh. Obshch. Khim.*, 1993, **63**, 1228; *J. Gen. Chem. USSR (Engl. Transl.)*, 1993, **63**, 857 (*amides, synth, pmr*)

2-(2-Fluorenyl)propanoic acid F-1-00006
α-Methyl-9H-fluorene-2-acetic acid, 9CI. Cicloprofen, BAN, INN, USAN. Cycloprofen. SQ 20824
[36950-96-6]



(R)-form

$C_{16}H_{14}O_2$ M 238.2
Analgesic, antiinflammatory agent. Never marketed.
(R)-form [54815-81-5]
Cryst. Mp 178-179°. $[\alpha]_D^{23}$ +56.
(S)-form [54815-83-7]
Cryst. Mp 179-181°. $[\alpha]_D^{23}$ −56.
(±)-form [54815-86-0]
Mp 181-183°.
Stiller, E.T. *et al, J. Med. Chem.*, 1972, **15**, 1029 (*synth, pharmacol*)
U.S. Pat., 3 856 977, (1974) (*ER Squibb*); *CA*, **82**, 125179q (*synth, resoln*)
Dean, A.V. *et al, Xenobiotica*, 1977, **7**, 549; 1978, **8**, 121 (*metab*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, London, 1982/1989, 2626.
Maitre, J.M. *et al, J. Chromatogr.*, 1984, **299**, 397 (*resoln*)
Singh, N.N. *et al, J. Chromatogr.*, 1986, **378**, 125 (*gc*)

2-Fluorobenzyl alcohol F-1-00007
2-Fluorobenzenemethanol, 9CI
[446-51-5]

C_7H_7FO M 126.1
d 1.17. Bp_{14} 94-96°. n_D^{20} 1.51.
[102606-96-2, 134430-68-5]
Shoesmith, J.B. *et al, J.C.S.*, 1926, 214 (*synth*)
Mamalis, P. *et al, J.C.S.*, 1965, 1829 (*synth*)
Tariq, S. *et al, Indian J. Phys., B*, 1983, **57**, 356 (*ir, Raman*)
Hansen, P.E. *et al, J. Magn. Reson.*, 1985, **62**, 487 (*F-19 nmr*)

3-Fluorobenzyl alcohol F-1-00008
3-Fluorobenzenemethanol, 9CI
[456-47-3]
C_7H_7FO M 126.1
d 1.16. Bp_{22} 104-105°.
4-Methylbenzenesulfonyl: [3821-46-3]. Mp 54.2-54.7°.
[102606-95-1]
Fang, F.T. *et al, J.A.C.S.*, 1958, **80**, 563 (*synth*)
Fukui, K. *et al, Nippon Kagaku Zasshi*, 1958, **79**, 1428; *CA*, **54**, 5518i (*synth*)

4-Fluorobenzyl alcohol F-1-00009
4-Fluorobenzenemethanol
[459-56-3]
C_7H_7FO M 126.1
d 1.16. Mp 22-23°. Bp_{730} 209°, Bp_1 59-59.5°.
4-Methylbenzenesulfonyl: [3859-77-6]. Mp 56.2-56.7°.
[659-46-1]
Fang, F.T. *et al, J.A.C.S.*, 1958, **80**, 563, 568 (*synth*)
Fukui, K. *et al, Nippon Kagaku Zasshi*, 1958, **79**, 1428; *CA*, **54**, 5518i (*synth*)
Balakrishnan, P. *et al, Tet. Lett.*, 1984, **25**, 169 (*O-17 nmr*)
Visser, T. *et al, Spectrochim. Acta A*, 1986, **42**, 599 (*ir, conformn*)

(2-Fluorobenzyl) triphenylphosphonium(1+) F-1-00010
[(2-Fluorophenyl)methyl] triphenylphosphonium(1+)

$C_{25}H_{21}FP^{\oplus}$ M 371.4 (ion)

Chloride: [106795-58-8].
$C_{25}H_{21}ClFP$ M 406.8 Rhombic prisms. Mp 298-300°.

[82757-27-5]

Fleming, I. *et al, J.C.S. Perkin 1*, 1986, 349 (*synth, pmr*)

(3-Fluorobenzyl) triphenylphosphonium(1+) F-1-00011

[(*3-Fluorophenyl*)*methyl*] *triphenylphosphonium(1+)*

$C_{25}H_{21}FP^{\oplus}$ M 371.4 (ion)

Bromide: [89302-81-8].
$C_{25}H_{21}BrFP$ M 451.3 Powder. Mp 309-310°.

Rafizadeh, K. *et al, J.O.C.*, 1984, **49**, 1500 (*synth, ir, pmr*)

Fluorobis(trifluoromethyl) arsine, 8CI F-1-00012

Bis(trifluoromethyl)arsinous fluoride, 9CI. Bis(trifluoromethyl)arsenic fluoride

[359-54-6]

$(F_3C)_2AsF$

C_2AsF_7 M 231.9
Synth. from $(F_3C)_3As + F_2$; $(F_3C)_2AsI + AgF$; or from $AsF_3 + Cd(CF_3)_2$. Liq. or gas. Bp 25° (extrap.), Bp_{232} 0°.

Walaschewski, E.J., *Chem. Ber.*, 1953, **86**, 272 (*synth*)
Emeléus, H.J. *et al, J.C.S.*, 1953, 1552 (*synth*)
Demuth, R., *Z. Anorg. Allg. Chem.*, 1975, **418**, 149 (*ir, Raman*)
Riesel, L. *et al, Z. Anorg. Allg. Chem.*, 1990, **588**, 26 (*synth*)

2-Fluoro-1,3-butadiene F-1-00013

Fluoroprene

[381-61-3]

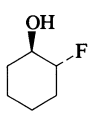
$H_2C{=}CFCH{=}CH_2$

C_4H_5F M 72.0
Antioxidant in polymers. Liq. or gas. Bp 12°. n_D 1.4010.

Orr, R.J. *et al, Can. J. Chem.*, 1955, **33**, 1328 (*synth*)
Petrow, A.A. *et al, Zh. Obshch. Khim.*, 1956, **26**, 3314; *J. Org. Chem. USSR (Engl. Transl.)*, 1956, **26**, 2452 (*synth*)
Fr. Pat., 1 486 739, (1967); *CA*, **68**, 79404v (*use*)
Tarasova, N.V. *et al, CA*, 1969, **42**, 1602 (*conformn*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, New York, 1978-1984, **3**, 128 (*use*)

2-Fluorocyclohexanol, 9CI F-1-00014

[656-60-0]



$C_6H_{11}FO$ M 118.1

(*1RS,2RS*)-*form* [14365-32-3]
(±)-trans-*form*
Mp 20-21°. Bp_{14} 68-69°.

Me ether: [65267-06-3]. *1-Fluoro-2-methoxycyclohexane, 9CI*
$C_7H_{13}FO$ M 132.1 Bp_{20} 45°.

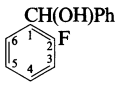
[20421-48-1, 65267-05-2, 79186-49-5, 98014-25-6]

Farges, G. *et al, Bull. Soc. Chim. Fr.*, 1963, 51 (*synth*)
Withig, G. *et al, Chem. Ber.*, 1963, **96**, 329 (*synth*)
Olah, G. *et al, Isr. J. Chem.*, 1978, **17**, 148 (*synth*)
Baklouti, A. *et al, J. Fluorine Chem.*, 1981, **18**, 45 (*synth, pmr, F-19 nmr, ms, deriv*)
Jones, P.G. *et al, Acta Cryst. C*, 1992, **48**, 852 (*cryst struct, derivs*)

2-Fluorodiphenylmethanol F-1-00015

2-Fluoro-α-phenylbenzenemethanol, 9CI. 2-Fluorobenzhydrol, 8CI

[362-54-9]



$C_{13}H_{11}FO$ M 202.2

(−)-*form* [143880-81-3]
Mp 47-48°. $[\alpha]_D$ −9.2 (c, 3.0 in Me_2CO).

(±)-*form*
Cubes. Mp 41-42°.

Bachmann, W.E. *et al, J.O.C.*, 1943, **8**, 320 (*synth*)
Brown, E. *et al, Tetrahedron: Asymmetry*, 1992, **3**, 841 (*synth*)

3-Fluorodiphenylmethanol F-1-00016

3-Fluoro-α-phenylbenzenemethanol. 3-Fluorobenzhydrol

[365-17-3]

$C_{13}H_{11}FO$ M 202.2

(±)-*form*
Solid or viscous liq. Mp 26-27°. Bp_{16} 178-179°.

Bachmann, W.E. *et al, J.O.C.*, 1943, **8**, 320 (*synth*)

4-Fluorodiphenylmethanol F-1-00017

4-Fluoro-α-phenylbenzenemethanol, 9CI. 4-Fluorobenzhydrol, 8CI

[365-22-0]

$C_{13}H_{11}FO$ M 202.2

(±)-*form*
Cryst. (hexane/Et_2O). Mp 48°. Bp_{16} 175-178°.

Koopal, S.A., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1915, **34**, 8, 158 (*synth*)
Schiemann, G. *et al, Ber.*, 1931, **64**, 1340 (*synth*)
Maruyama, K. *et al, J. Phys. Org. Chem.*, 1991, **4**, 501 (*synth, ms*)
Rieke, R. *et al, Synth. Commun.*, 1994, **24**, 2379 (*ir, pmr, cmr*)

1-Fluoroethanol, 9CI F-1-00018

[40017-45-6]

$H_3CCHFOH$

C_2H_5FO M 64.0

(±)-*form*

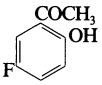
Ac:
$C_4H_7FO_2$ M 106.0 Liq. Bp 90-91°. n_D^{20} 1.3766.

Limat, D. *et al, Annalen*, 1995, 849.

5′-Fluoro-2′-hydroxyacetophenone F-1-00019

1-(5-Fluoro-2-hydroxyphenyl)ethanone, 9CI. 2-Acetyl-4-fluorophenol

[394-32-1]



$C_8H_7FO_2$ M 154.1
Mp 56-58°. Bp_8 65-66°.

Joshi, K.C. *et al, J. Indian Chem. Soc.*, 1962, **39**, 185 (*synth*)
Givens, E.N. *et al, J. Chem. Eng. Data*, 1969, **14**, 392 (*pmr, ms*)

3-Fluoro-2-hydroxybenzaldehyde F-1-00020

1-Fluoro-6-formylphenol. 3-Fluorosalicylaldehyde

[394-50-3]

$C_7H_5FO_2$ M 140.1
Mp 68-70°.

2,4-Dinitrophenylhydrazone: Orange needles (EtOH). Mp 282-283°.
Me ether: [74266-68-5]. *3-Fluoro-2-methoxybenzaldehyde. 1-Fluoro-3-formyl-2-methoxybenzene. 3-Fluoro-o-anisaldehyde*
$C_8H_7FO_2$ M 154.1 Mp 47-48°. Bp_{12} 82°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1295A.
Ferguson, L.N. *et al, J.A.C.S.*, 1946, **68**, 2502.
U.S. Pat., 4 124 643, (1978); *CA*, **90**, 87041 (*synth*)
Aymes, D.J. *et al, Bull. Soc. Chim. Fr.*, 1980, 175 (*synth*)
Ladd, D.L. *et al, Synth. Commun.*, 1985, **15**, 61 (*deriv*)
Furlano, D.C. *et al, J.O.C.*, 1988, **53**, 3145 (*deriv*)

3-Fluoro-4-hydroxybenzaldehyde F-1-00021

$C_7H_5FO_2$ M 140.1
Needles (H_2O). Mp 121-122°.

Oxime:
$C_7H_6FNO_2$ M 155.1 Cryst. (H_2O). Mp 140-141°.

2,4-Dinitrophenylhydrazone: Scarlet needles. Mp 291-292°.

Ferguson, L.N. *et al, J.A.C.S.*, 1946, **68**, 2502.

5-Fluoro-2-hydroxybenzaldehyde F-1-00022

5-Fluorosalicylaldehyde

[347-54-6]

$C_7H_5FO_2$ M 140.1
Plates. Mp 82-84°.

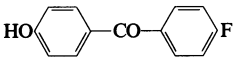
Phenylhydrazone: Yellow plates. Mp 144-145°.
2,4-Dinitrophenylhydrazone: Orange needles. Mp 285-287°.
Me ether: [19415-51-1]. *5-Fluoro-2-methoxybenzaldehyde*
$C_8H_7FO_2$ M 154.1 Mp 43-45.5°.

Ferguson, L.N. *et al*, *J.A.C.S.*, 1946, **68**, 2502.
Misaki, S., *J. Fluorine Chem.*, 1982, **21**, 191.
Vallgårda, J. *et al*, *J.C.S. Perkin 1*, 1994, 461.
Aldred, R. *et al*, *J.C.S. Perkin 1*, 1994, 1823 (*synth, pmr*)

4-Fluoro-4′-hydroxybenzophenone F-1-00023

(*4-Fluorophenyl*)(*4-hydroxyphenyl*)*methanone, 9CI*

[25913-05-7]



$C_{13}H_9FO_2$ M 216.2
Cryst. (EtOH aq.). Mp 170-172°.

Me ether: [345-89-1]. *4-Fluoro-4′-methoxybenzophenone*
$C_{14}H_{11}FO_2$ M 230.2 Cryst. (EtOH). Mp 97° (94°). $Bp_{1.1\text{-}1.5}$ 148-152°.

Me ether, 2,4-dinitrophenylhydrazone: Mp 227-228°.

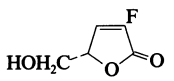
Ph ether: [16574-56-4]. *4-Fluoro-4′-phenoxybenzophenone*
$C_{19}H_{13}FO_2$ M 292.3 Cryst. (EtOH). Mp 101.5° (99°). $Bp_{0.38}$ 180-182°.

[76597-40-5, 88164-67-4]

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1273A.
Dayal, S.K. *et al*, *J.A.C.S.*, 1972, **94**, 9113 (*F-19 nmr, deriv*)
Shapiro, M.J., *Tetrahedron*, 1977, **33**, 1091 (*cmr, deriv*)
Ridd, J.H. *et al*, *J.C.S. Perkin 2*, 1988, 1729 (*synth*)

3-Fluoro-5-(hydroxymethyl)-2(5*H*)-furanone, 9CI F-1-00024

2-Fluoro-4-(hydroxymethyl)-2-buten-4-olide



(*S*)-*form*

$C_5H_5FO_3$ M 132.0

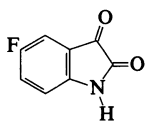
(***S*)-*form*** [154540-16-6]
Oil. $[\alpha]_D^{23}$ −28.5 (c, 1 in $CHCl_3$).

Patrick, T.B. *et al*, *J.O.C.*, 1994, **59**, 1210 (*synth, pmr, F-19 nmr*)

5-Fluoro-1*H*-indole-2,3-dione, 9CI F-1-00025

5-Fluoroisatin

[443-69-6]



$C_8H_4FNO_2$ M 165.1
Brick-red needles (AcOH aq.). Mp 227°.

3-Oxime: [319-64-2].
$C_8H_5FN_2O_2$ M 180.1 Mp 202-204°.

Yen, V.Q. *et al*, *J.O.C.*, 1958, **23**, 1858 (*synth*)
Castle, R.N. *et al*, *J. Het. Chem.*, 1965, **2**, 459 (*synth*)
Kearney, T. *et al*, *Synthesis*, 1992, 769 (*3-oxime*)

3-Fluoro-6-iodopyridazine, 9CI F-1-00026

[162438-03-1]

$C_4H_2FIN_2$ M 223.9
Tan solid. Mp 118-120°.

Draper, T.L. *et al*, *J.O.C.*, 1995, **60**, 748 (*synth, pmr*)

3-Fluoro-2-iodo-4-pyridinecarboxylic acid, 9CI F-1-00027

[153035-09-7]

$C_6H_3FINO_2$ M 266.9
Cryst. by subl. Mp 220° subl. $Subl._1$ 140°.

Rocca, P. *et al*, *J.O.C.*, 1993, **58**, 7832 (*synth, pmr, cmr, ir*)

1-Fluoro-4-(isothiocyanatomethyl)benzene, 9CI F-1-00028

4-Fluorobenzylisothiocyanate

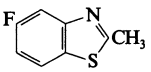
[2740-88-7]

C_8H_6FNS M 167.2
Bp_9 122-124°.

Cherbuliez, E. *et al*, *Helv. Chim. Acta*, 1965, **48**, 1031 (*synth*)

5-Fluoro-2-methylbenzothiazole F-1-00029

[399-75-7]



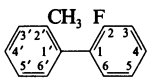
C_8H_6FNS M 167.2
d 1.26. Bp_7 110-112°.

[86701-25-9]

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1512A.
Kiprianov, A.I. *et al*, *Zh. Obshch. Khim.*, 1952, **22**, 2209 (*synth*)
Bassignana, P. *et al*, *Spectrochim. Acta*, 1963, **19**, 1885 (*ir*)
Sawhney, S.N. *et al*, *J.O.C.*, 1979, **44**, 1136 (*cmr*)

2-Fluoro-2′-methylbiphenyl F-1-00030

[80254-69-9]



$C_{13}H_{11}F$ M 186.2
Identified spectroscopically.

Kelm, J. *et al*, *Spectrochim. Acta A*, 1981, **37**, 689 (*synth, F-19 nmr*)
Herman, E.C. *et al*, *Spectrochim. Acta A*, 1982, **38**, 1057 (*F-19 nmr*)

2-Fluoro-3-methylbiphenyl F-1-00031

[82617-47-8]

$C_{13}H_{11}F$ M 186.2

U.S. Pat., 4 402 973, (1983); *CA*, **100**, 68561x (*synth*)

2-Fluoro-3′-methylbiphenyl F-1-00032

[76350-77-1]

$C_{13}H_{11}F$ M 186.2
Identified spectroscopically.

Kelm, J. *et al*, *Spectrochim. Acta A*, 1981, **37**, 689 (*synth, F-19 nmr*)
Herman, E.C. *et al*, *Spectrochim. Acta A*, 1982, **38**, 1057 (*F-19 nmr*)

2-Fluoro-4-methylbiphenyl F-1-00033

[69168-29-2]

$C_{13}H_{11}F$ M 186.2

Eur. Pat., 117 631, (1984); *CA*, **102**, 212787m (*synth*)

2-Fluoro-4′-methylbiphenyl F-1-00034

[72093-41-5]

$C_{13}H_{11}F$ M 186.2
Identified spectroscopically.

Kelm, J. *et al*, *Spectrochim. Acta A*, 1981, **37**, 689 (*synth, F-19 nmr*)
Hermann, E.C. *et al*, *Spectrochim. Acta A*, 1982, **38**, 1057 (*F-19 nmr*)

3-Fluoro-2-methylbiphenyl F-1-00035

$C_{13}H_{11}F$ M 186.2
Yellow liq. $Bp_{1.2}$ 88-90°, $Bp_{0.5}$ 74-77°.

Smith, G.G. *et al*, *J.A.C.S.*, 1960, **82**, 99 (*synth*)

3′-Fluoro-2-methylbiphenyl F-1-00036

[80254-70-2]

$C_{13}H_{11}F$ M 186.2
Identified spectroscopically.

Kelm, J. *et al*, *Spectrochim. Acta A*, 1981, **37**, 689 (*synth, F-19 nmr*)
Hermann, E.C. *et al*, *Spectrochim. Acta A*, 1982, **38**, 1057 (*F-19 nmr*)

3-Fluoro-3′-methylbiphenyl F-1-00037

[80254-71-3]

$C_{13}H_{11}F$ M 186.2
Identified spectroscopically.

Kelm, J. *et al*, *Spectrochim. Acta A*, 1981, **37**, 689 (*synth, F-19 nmr*)
Hermann, E.C. *et al*, *Spectrochim. Acta A*, 1982, **38**, 1057 (*F-19 nmr*)

3-Fluoro-4-methylbiphenyl, 9CI F-1-00038

[135227-04-2]

$C_{13}H_{11}F$ M 186.2
Oil.

Lipshutz, B.H. *et al*, *J.A.C.S.*, 1993, **115**, 9276 (*synth, ir, pmr, cmr*)

3-Fluoro-4′-methylbiphenyl F-1-00039

[72093-42-6]

$C_{13}H_{11}F$ M 186.2
Identified spectroscopically.

Kelm, J. *et al*, *Spectrochim. Acta A*, 1981, **37**, 689 (*synth, F-19 nmr*)
Hermann, E.C. *et al*, *Spectrochim. Acta A*, 1982, **38**, 1057 (*F-19 nmr*)

4′-Fluoro-2-methylbiphenyl F-1-00040

[72968-86-6]

$C_{13}H_{11}F$ M 186.2
$Bp_{0.8}$ 90-93°.

Bell, H.C. *et al*, *Aust. J. Chem.*, 1979, **32**, 1531 (*synth, uv, pmr, ms*)
Kelm, J. *et al*, *Spectrochim. Acta A*, 1981, **37**, 689 (*synth, F-19 nmr*)
Hermann, E.C. *et al*, *Spectrochim. Acta A*, 1982, **38**, 1057 (*F-19 nmr*)

4′-Fluoro-3-methylbiphenyl F-1-00041

[10540-44-0]

$C_{13}H_{11}F$ M 186.2
$Bp_{0.4}$ 87-92°. $n_D^{24.5}$ 1.5730.

Kelm, J. *et al*, *Spectrochim. Acta A*, 1981, **37**, 689 (*synth, F-19 nmr*)
Hermann, E.C. *et al*, *Spectrochim. Acta A*, 1982, **38**, 1057 (*F-19 nmr*)
Brune, H.A. *et al*, *Z. Naturforsch., B*, 1984, **39**, 1772 (*synth, ir, pmr, ms*)

4-Fluoro-4′-methylbiphenyl F-1-00042

[72093-43-7]

$C_{13}H_{11}F$ M 186.2
Mp 77-78° (64°).

Bell, H.C. *et al*, *Aust. J. Chem.*, 1979, **32**, 1531 (*synth, uv, pmr, ms*)
Hermann, E.C. *et al*, *Spectrochim. Acta A*, 1982, **38**, 1057 (*F-19 nmr*)
Brune, H.A. *et al*, *Z. Naturforsch., B*, 1984, **39**, 1772 (*synth, ir, pmr, ms*)

(Fluoromethyl) diphenylphosphine F-1-00043

Ph_2PCH_2F

$C_{13}H_{12}FP$ M 218.2

Oxide: [131581-39-0].
$C_{13}H_{12}FOP$ M 234.2 Wittig-Horner reagent for synth. of fluoroalkenes from carbonyl compds. Solid. Mp 93-94°.

Edwards, M.L. *et al*, *Tet. Lett.*, 1990, **31**, 5571 (*synth, pmr, F-19 nmr, use*)

2-Fluoro-2-methyl-1-propanol, 9CI F-1-00044

[3109-99-7]

$(H_3C)_2CFCH_2OH$

C_4H_9FO M 92.1
Liq. Bp 116-118°. n_D^{20} 1.3975.

Ac:
$C_6H_{11}FO_2$ M 134.1 Liq. Bp_{10} 58-59°. n_D^{20} 1.3863.

Farges, G. *et al*, *Bull. Soc. Chim. Fr.*, 1963, 51 (*synth*)
Wiechert, K. *et al*, *Z. Chem.*, 1965, **5**, 380 (*synth*)
Limat, D. *et al*, *Annalen*, 1995, 849 (*Ac*)

1-Fluoro-4-nitro-2-(trifluoromethyl)benzene, 9CI F-1-00045

α,α,α,2-Tetrafluoro-5-nitrotoluene. 2-Fluoro-5-nitrobenzotrifluoride

[400-74-8]

$C_7H_3F_4NO_2$ M 209.1
d 1.52. Bp_{25} 105-110°, $Bp_{4.5}$ 77-79°.

Finger, G.C. *et al*, *J.A.C.S.*, 1956, **78**, 6034 (*synth*)
Maggini, M. *et al*, *J.O.C.*, 1991, **56**, 6406 (*synth*)

1-Fluoro-4-nitro-3-(trifluoromethyl)benzene F-1-00046

α,α,α,3-Tetrafluoro-6-nitrotoluene. 5-Fluoro-2-nitrobenzotrifluoride

$C_7H_3F_4NO_2$ M 209.1
Liq. Bp 198-199°.

Finger, G.C. *et al*, *J.A.C.S.*, 1944, **66**, 1972 (*synth*)

2-Fluoro-9-octadecenoic acid, 9CI F-1-00047

$H_3C(CH_2)_7CH{=}CH(CH_2)_6CHFCOOH$

$C_{18}H_{33}FO_2$ M 300.4

(±)-(*Z*)-*form* [155056-28-3]
Cryst. (pentane). Mp 40.5-41.5°.

Oliver, J.E. *et al*, *Synthesis*, 1994, 273 (*synth, pmr, cmr, ms*)

4-Fluorooctanoic acid F-1-00048

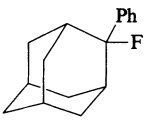
$H_3C(CH_2)_3CHFCH_2CH_2COOH$

$C_8H_{15}FO_2$ M 162.2

(±)-*form*
Oil.

Nagatsugi, F. *et al*, *Chem. Pharm. Bull.*, 1995, **43**, 607 (*synth*)

2-Fluoro-2-phenyladamantane F-1-00049



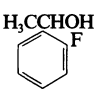
$C_{16}H_{19}F$ M 230.3
Solid.

Laube, T. *et al*, *Helv. Chim. Acta*, 1994, **77**, 1773 (*synth, pmr, F-19 nmr*)

1-(2-Fluorophenyl)ethanol F-1-00050

2-Fluoro-α-methylbenzenemethanol, 9CI. 2-Fluoro-α-methylbenzyl alcohol, 8CI

[445-26-1]



C_8H_9FO M 140.1
Liq. Bp_{40} 113-114°.

[155671-20-8]

Sianesi, D., *Gazz. Chim. Ital.*, 1959, **89**, 1749 (*synth*)
Buu-Hoi, N.P. *et al*, *J.O.C.*, 1962, **27**, 2669 (*synth*)

1-(3-Fluorophenyl)ethanol F-1-00051

3-Fluoro-α-methylbenzenemethanol, 9CI. 3-Fluoro-α-methylbenzyl alcohol, 8CI

[402-63-1]

C_8H_9FO M 140.1
Liq. Bp_{10} 104-106°.

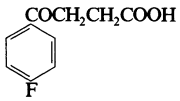
[126534-32-5, 126534-33-6, 147164-51-0]

Sianesi, D., *Gazz. Chim. Ital.*, 1959, **89**, 1749 (*synth*)

4-(4-Fluorophenyl)-4-oxobutanoic acid F-1-00052

4-Fluoro-γ-oxobenzenebutanoic acid, 9CI. 3-(4-Fluorobenzoyl)propionic acid, 8CI

[366-77-8]



$C_{10}H_9FO_3$ M 196.1
Cryst. (EtOH). Mp 100-102°.

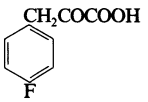
Et ester: [41310-80-9].
$C_{12}H_{13}FO_3$ M 224.2 Cryst. (C_6H_6/petrol). Mp 46-49°.

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 157C.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 144C.
Adcock, W. *et al*, *J.A.C.S.*, 1967, **89**, 386 (*synth*)
Sindelar, K. *et al*, *Coll. Czech. Chem. Comm.*, 1973, **38**, 3879 (*synth, pmr, ester*)

3-(4-Fluorophenyl)-2-oxopropanoic acid F-1-00053

4-Fluoro-α-oxobenzenepropanoic acid

[7761-30-0]



$C_9H_7FO_3$ M 182.1

Et ester:
$C_{11}H_{11}FO_3$ M 210.2 Liq.

Schuster, H.F. *et al*, *J. Het. Chem.*, 1994, **31**, 1381 (*synth, ir, pmr*)

2-Fluoropropanoic acid, 9CI F-1-00054

[6087-13-4]

$H_3CCHFCOOH$

$C_3H_5FO_2$ M 92.0

(±)-*form*
Liq. Bp 163°. Strongly hydrophilic; difficult to sep. from aq. solns.

Me ester: [94726-03-1].
$C_4H_7FO_2$ M 106.0 Liq. Bp 106.5-108.5°.

Et ester: [127306-59-6].
$C_5H_9FO_2$ M 120.1 Liq. Bp 122.5-123°.

Chloride: [159249-10-2].
C_3H_4ClFO M 110.5 Liq. Bp 80.5-81°.

Amide: [430-98-8].
C_3H_6FNO M 91.0 Cryst. Mp 75-76°.

Nitrile: [814-65-3]. *1-Cyano-1-fluoroethane*
C_3H_4FN M 73.0 Liq. Bp 83-83.5°.

[349-43-9, 430-97-7, 2366-56-5, 57965-29-4, 72959-94-5, 72959-95-6, 75244-22-3]

Gryszkiewicz-Trochimowski, E. *et al*, *Bull. Soc. Chim. Fr.*, 1949, 928 (*synth*)
Olah, G.A. *et al*, *Synthesis*, 1974, 652 (*synth*)
O'Hagon, D., *J. Fluorine Chem.*, 1989, **43**, 371 (*synth*)
Sierra, T. *et al*, *J.A.C.S.*, 1992, **114**, 7645 (*synth, ir, pmr*)
Fritz-Langhals, E. *et al*, *Tet. Lett.*, 1993, **34**, 293 (*synth, ir, pmr*)

1-Fluorotetradecane, 9CI F-1-00055

Tetradecyl fluoride

[593-33-9]

$H_3C(CH_2)_{12}CH_2F$

$C_{14}H_{29}F$ M 216.3
d 0.83. Bp_2 120.4°. n_D^{20} 1.4264.

Macey, W.A.T., *J. Phys. Chem.*, 1960, **64**, 254 (*synth*)
Watanabe, S. *et al*, *J. Am. Oil Chem. Soc.*, 1983, **60**, 1678; *CA*, **100**, 22317u (*synth*)
Crowder, G.A. *et al*, *J. Mol. Struct.*, 1983, **99**, 77 (*ir*)
Shimizu, M. *et al*, *Tet. Lett.*, 1985, **26**, 4207 (*synth*)

2-Fluoro-3-(trifluoromethyl) aniline F-1-00056

2-Fluoro-3-(trifluoromethyl)benzenamine, 9CI. 3-Amino-2-fluorobenzotrifluoride. α,α,α,2-Tetrafluoro-m-toluidine

[123973-25-1]

$C_7H_5F_4N$ M 179.1
d 1.39. n_D^{20} 1.46.

Ger. Pat., 3 737 9866, (1989) (*Bayer*); *CA*, **111**, 232267f (*synth*)

2-Fluoro-5-(trifluoromethyl) aniline F-1-00057

3-Amino-4-fluorobenzotrifluoride. α,α,α,6-Tetrafluoro-m-toluidine. 2-Fluoro-5-(trifluoromethyl)benzenamine, 9CI

[535-52-4]

$C_7H_5F_4N$ M 179.1
d 1.38. Bp 188-190°, Bp_{20} 81°. n_D^{20} 1.46.

Brown, J.H. *et al*, *J.C.S.*, 1949, 595, 599 (*synth*)
Finger, G.C. *et al*, *J.A.C.S.*, 1956, **78**, 6034, 6037 (*synth*)
Fifolt, M.J. *et al*, *J.O.C.*, 1989, **54**, 3019 (*F-19 nmr*)

4-Fluoro-2-(trifluoromethyl) aniline F-1-00058

4-Fluoro-2-(trifluoromethyl)benzenamine, 9CI. α,α,α,4-Tetrafluoro-o-toluidine. 2-Amino-5-fluorobenzotrifluoride

[393-39-5]

$C_7H_5F_4N$ M 179.1
d 1.38. $Bp_{17.5}$ 70-72°, Bp_{40} 89-90°.

N-*Ac:*
$C_9H_7F_4NO$ M 221.1 Needles (EtOH aq.). Mp 121-121.5°.

Finger, G.C. *et al*, *J.A.C.S.*, 1944, **66**, 1972.
Mulvey, D.M. *et al*, *Tet. Lett.*, 1978, 1419 (*synth*)
Fifolt, M.J. *et al*, *J.O.C.*, 1989, **54**, 3019 (*F-19 nmr*)

5-Fluoro-2-(trifluoromethyl) aniline F-1-00059

5-Fluoro-2-(trifluoromethyl)benzenamine, 9CI. α,α,α,5-Tetrafluoro-o-toluidine, 8CI. 2-Amino-4-fluorobenzotrifluoride

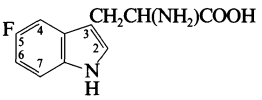
$C_7H_5F_4N$ M 179.1

N-*Ac:*
$C_9H_7F_4NO$ M 221.1 Mp 91-92°.

Yagupol'skii, L.M. *et al*, *Zh. Obshch. Khim.*, 1963, **33**, 2358; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1963, **33**, 2297 (*synth*)

5-Fluorotryptophan, 9CI F-1-00060

[343-91-9]



$C_{11}H_{11}FN_2O_2$ M 222.2
(±)-***form*** [154-08-5]
Cryst. Mp 265° dec.

[16626-02-1, 97749-24-1]

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 672D.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 540C.
Hoffman, E. *et al*, *J. Het. Chem.*, 1965, **2**, 298 (*synth*)
Bentov, M. *et al*, *Isr. J. Chem.*, 1969, **7**, 835 (*synth*)

6-Fluorotryptophan, 9CI F-1-00061

[343-92-0]

$C_{11}H_{11}FN_2O_2$ M 222.2
(±)-***form*** [7730-20-3]
Cryst. Mp 280-285° dec.

[19310-00-0, 108391-82-8]

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 672C.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 540B.
Bergmann, E.D. *et al*, *J.C.S.*, 1962, 2827 (*synth*)
Bentov, M. *et al*, *Isr. J. Chem.*, 1969, **7**, 835 (*synth*)

2-Fluoroundecanoic acid, 9CI F-1-00062

[10457-83-7]

$H_3C(CH_2)_8CHFCOOH$

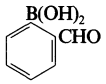
$C_{11}H_{21}FO_2$ M 204.2
(±)-***form*** [155056-26-1]
Cryst. (pentane or Me_2CO aq.). Mp 64-64.5° (61-62°).

Gershon, H. *et al*, *J. Med. Chem.*, 1967, **10**, 186 (*synth*)
Oliver, J.E. *et al*, *Synthesis*, 1994, 273 (*synth, pmr, cmr, ms*)

(2-Formylphenyl)boronic acid, 9CI F-1-00063

o-Formylbenzeneboronic acid, 8CI. (2-Formylphenyl)dihydroxyborane

[40138-16-7]



$C_7H_7BO_3$ M 149.9
Benzodiazaborine derivs. prepd. from the title compd. have bactericidal props. Needles (H_2O); cryst. ($MeNO_2$). Spar. sol. CCl_4, cyclohexane; mod. sol. toluene; v. sol. hot H_2O. Mp 118-120° dec. (dehydrates), Mp 163-165° (double Mp).

Torssell, K., *Ark. Kemi*, 1957, **10**, 507 (*synth*)
Snyder, H.R. *et al*, *J.A.C.S.*, 1958, **80**, 835 (*synth*)
Tschampel, P. *et al*, *J.O.C.*, 1964, **29**, 2168 (*synth*)
Ger. Pat., 1 670 494, (1976); *CA*, **86**, 90009n (*synth*)
Ger. Pat., 2 533 918, (1977); *CA*, **87**, 23334x (*synth*)
U.S. Pat., 4 199 573, (1980); *CA*, **93**, 186544d (*synth*)
Yang, Y. *et al*, *J. Het. Chem.*, 1989, **26**, 865 (*props*)
Wytko, J.A. *et al*, *J.O.C.*, 1992, **57**, 1017 (*synth, pmr*)
Scouten, W.H. *et al*, *J. Chem. Crystallogr.*, 1994, **24**, 621 (*synth, pmr, cryst struct*)

(3-Formylphenyl)boronic acid F-1-00064

m-*Formylbenzeneboronic acid. (3-Formylphenyl)dihydroxyborane*

[87199-16-4]

$C_7H_7BO_3$ M 149.9
Cryst. (H_2O). Mp 112° dec. (dehydrates), Mp 180° approx. (double Mp).

Torssell, K., *Ark. Kemi*, 1957, **10**, 507 (*synth*)

(4-Formylphenyl)boronic acid F-1-00065

p-*Formylbenzeneboronic acid. (4-Formylphenyl)dihydroxyborane*

[87199-17-5]

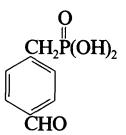
$C_7H_7BO_3$ M 149.9
Pale yellow needles (H_2O or MeCN). Mp 255-260°.

Torssell, K., *Ark. Kemi*, 1957, **10**, 507 (*synth*)
Snyder, H.R. *et al*, *J.A.C.S.*, 1958, **80**, 835 (*synth*)
Feulner, H. *et al*, *Chem. Ber.*, 1990, **123**, 1841 (*synth, ir, cryst struct*)
Jendralla, H. *et al*, *Annalen*, 1995, 1253 (*synth, ms*)

[(4-Formylphenyl)methyl] phosphonic acid F-1-00066

p-*Formylbenzylphosphonic acid*

[114496-50-3]

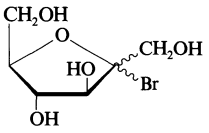


$C_8H_9O_4P$ M 200.1

Di-tert-*butyl ester:* [132541-47-0]. *Di*-tert-*butyl* [(*4-formylphenyl*)*methyl*]*phosphonate*. *4*-[[*Di*(tert-*butoxy*)*phosphinyl*]*methyl*] *benzaldehyde*
$C_{16}H_{25}O_4P$ M 312.3 Cryst. (petrol). Mp 60-63.5°.

Burke, T.R. *et al, J. Med. Chem.*, 1991, **34**, 1577 (*ester, synth, pmr*)
Burke, T.R. *et al, J.O.C.*, 1993, **58**, 1336 (*ester*)

Fructofuranosyl bromide F-1-00067



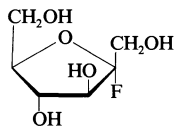
$C_6H_{11}BrO_5$ M 243.0

D-form

Tetrabenzoyl: [54401-13-7].
$C_{34}H_{27}BrO_9$ M 659.4 Syrup. $[\alpha]_D^{20}$ +40.3 ($CHCl_3$).

Helferich, B. *et al, Chem. Ber.*, 1953, **86**, 651 (*tetrabenzoyl*)
Hrebabecky, H. *et al, Coll. Czech. Chem. Comm.*, 1974, **39**, 2115 (*tetrabenzoyl*)
Chretien, F. *et al, J.C.S. Perkin 1*, 1988, 3297 (*use*)

Fructofuranosyl fluoride F-1-00068



α-D-*form*

$C_6H_{11}FO_5$ M 182.1

α-D-form

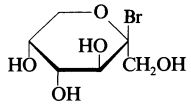
Tetra-Ac: [58634-84-7].
$C_{14}H_{19}FO_9$ M 350.2 Syrup. $[\alpha]_D^{22}$ +45 ($CHCl_3$).

β-D-form

Tetra-Ac: [475-02-5].
Syrup. $[\alpha]_D^{22}$ +36 ($CHCl_3$).

Erbing, B. *et al, Acta Chem. Scand., Ser. B*, 1976, **30**, 12 (*tetra-Ac, cmr*)

Fructopyranosyl bromide F-1-00069



$C_6H_{11}BrO_5$ M 243.0

β-D-form

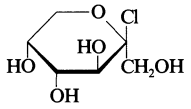
Tetra-Ac: [14218-13-4].
$C_{14}H_{19}BrO_9$ M 411.2 Cryst. (Et_2O). Mp 65°. $[\alpha]_D^{20}$ −189.1 ($CHCl_3$).

1,4,5-Tribenzoyl, 3-mesyl:
$C_{28}H_{25}BrO_{10}S$ M 633.4 Cryst. (Et_2O/pentane). Mp 157-158° dec. $[\alpha]_D^{20}$ −207 (c, 0.96 in CH_2Cl_2).

Tetrakis(p-*nitrobenzoyl*): [70551-21-2].
Cryst. (Et_2O/$CHCl_3$). Mp 162-163°. $[\alpha]_D^{25}$ −170 (c, 1.2 in $CHCl_3$).

Brauns, D.H. *et al, J.A.C.S.*, 1923, **45**, 2381 (*β-tetra-Ac*)
Yamana, S. *et al, J.O.C.*, 1966, **31**, 3698 (*β-tetra-Ac*)
Ness, R.K. *et al, J.O.C.*, 1968, **33**, 181 (*β-tribenzoyl*)
Steinlin, H. *et al, Helv. Chim. Acta*, 1979, **62**, 378 (*β-tetranitrobenzoyl, pmr, cmr*)

Fructopyranosyl chloride F-1-00070



$C_6H_{11}ClO_5$ M 198.6

β-D-form

Tetra-Ac: [14262-86-3].
$C_{14}H_{19}ClO_9$ M 366.7 Cryst. (EtOH). Mp 108°. $[\alpha]_D^{20}$ +45.3 ($CHCl_3$).

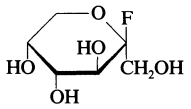
1,4,5-Tribenzoyl, 3-mesyl: [15080-06-5].
$C_{28}H_{25}ClO_{10}S$ M 589.0 Cryst. (Et_2O/pentane). Mp 161-163°. $[\alpha]_D^{20}$ −178 (c, 0.98 in CH_2Cl_2).

Tetrabenzoyl: [70551-23-4].
$C_{34}H_{27}ClO_9$ M 615.0 Liq. $[\alpha]_D^{25}$ −149.6 (c, 1.3 in $CHCl_3$).

Tetrakis(p-*nitrobenzoyl*): [70551-20-1].
Cryst. (CH_2Cl_2/Et_2O). Mp 200-203°. $[\alpha]_D^{25}$ −193 (c, 1 in $CHCl_3$).

Brauns, D.H. *et al, J.A.C.S.*, 1920, **42**, 1846 (*β-tetra-Ac*)
Ness, R.K. *et al, J.O.C.*, 1968, **33**, 181 (*β-tribenzoyl*)
Steinlin, H. *et al, Helv. Chim. Acta*, 1979, **62**, 378 (*β-tetrabenzoyl, ir, pmr, cmr*)

Fructopyranosyl fluoride F-1-00071



$C_6H_{11}FO_5$ M 182.1

β-D-form

Tetra-Ac: [2823-45-2].
$C_{14}H_{19}FO_9$ M 350.2 Cryst. (EtOH). V. sol. $CHCl_3$; spar. sol. EtOH, petrol. Mp 112°. $[\alpha]_D^{20}$ −90.4 ($CHCl_3$). Stable at r.t.

Brauns, D.H. *et al, J.A.C.S.*, 1923, **45**, 2381 (*β-tetra-Ac*)
Yamana, S. *et al, J.O.C.*, 1966, **31**, 3698 (*β-tetra-Ac*)

3-Furanacetic acid F-1-00072

[123617-80-1]
$C_6H_6O_3$ M 126.1
Translucent plates (petrol). Mp 61.9-62.2°.

Et ester: [57393-62-1].
$C_8H_{10}O_3$ M 154.1 Bp_{12} 83-85°.

Chloride:
$C_6H_5ClO_2$ M 144.5 Bp_3 53°.

Amide:
$C_6H_7NO_2$ M 125.1 Feathery needles (C_6H_6/petrol). Mp 114-115°.

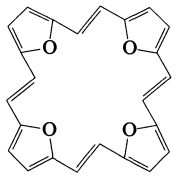
Nitrile: [68913-67-7]. *3-(Cyanomethyl)furan*
C_6H_5NO M 107.1 Bp_{19} 90-92°, $Bp_{0.4}$ 46°. n_D^{17} 1.4733.

[62689-88-7]

Sherman, E. *et al, J.A.C.S.*, 1950, **72**, 2195 (*synth, chloride, amide*)
Pelletier, S.W. *et al, Tetrahedron*, 1975, **31**, 1659 (*ester, ir, pmr, ms*)
Arena, G. *et al, J.C.S. Perkin 2*, 1993, 1941 (*nitrile*)

[2.2.2.2](2,5)-Furanophanetetraene F-1-00073

25,26,27,28-Tetraoxapentacyclo[*20.2.1.1*^{4,7}.*1*^{10,13}.*1*^{16,19}] *octacosa-2,4,6,8,10,12,14,16,18,20,22,24-dodecaene, 9CI.* [*24*]*Annulene tetroxide. Tetraoxaporphyrinogen*[*2.2.2.2*]



(*E,E,E,E*)-*form*

$C_{24}H_{16}O_4$ M 368.3

(E,E,E,E)-form
Violet prisms. Mp 269-270°.

(E,E,E,Z)-form
Violet-black prisms. Mp 215-217°.

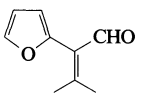
(E,Z,E,Z)-form [157750-37-3]
Black-violet cryst. Mp >300°. Air-stable. Forms the dication on oxidation.

Bis(*perchlorate*): [157643-31-7].
Microcrystalline blue powder with metallic sheen. Mp >300° dec.

Elix, J.A., *Aust. J. Chem.*, 1969, **22**, 1951 (*synth, uv*)
Märkl, G. *et al, Angew. Chem., Int. Ed.*, 1994, **33**, 1151 (*synth, uv, pmr, cmr, cryst struct*)

2-(2-Furanyl)-3-methyl-2-butenal F-1-00074

α-(*1-Methylethylidene*)-*2-furanacetaldehyde, 9CI.* α-*Isopropylidene-2-furanacetaldehyde*
[31681-28-4]



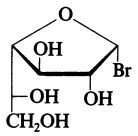
$C_9H_{10}O_2$ M 150.1
Constit. of the oil of *Papaver somniferum*. Yellow liq. Bp_5 89°.

Semicarbazone: [31681-29-5].
Mp 170°. Subl. 164°.

Dana, G. *et al, Bull. Soc. Chim. Fr.*, 1970, 3994 (*synth*)
Li, C. *et al, CA*, 1993, **118**, 165179 (*isol*)

G

Galactofuranosyl bromide G-1-00001



α-D-*form*

$C_6H_{11}BrO_5$ M 243.0

α-D-form

2,3-Dibenzoyl, 5-chloroacetyl, 6-pivaloyl: [127501-12-6].
$C_{27}H_{28}BrClO_9$ M 611.8 Oil. Unstable at ambient temp.

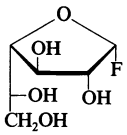
β-D-form

Tetra-Ac: [39698-24-3].
$C_{14}H_{19}BrO_9$ M 411.2 Oil.

2,3-Di-O-benzyl, 5,6-bis-(4-nitrobenzoyl): [55656-71-8].
$C_{34}H_{29}BrN_2O_{11}$ M 721.5 Amorph. solid. $[\alpha]_D^{25}$ −59.4 (c, 1.2 in $CHCl_3$).

Bock, K. *et al, Acta Chem. Scand., Ser. B*, 1974, **28**, 1041 (*β-tetra-Ac*)
Frechet, J.M.J. *et al, Can. J. Chem.*, 1975, **53**, 670 (*β-deriv*)
Veeneman, G.H. *et al, Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1989, **108**, 344 (*α-deriv, pmr, cmr*)

Galactofuranosyl fluoride G-1-00002



α-D-*form*

$C_6H_{11}FO_5$ M 182.1

α-D-form

Tetra-Ac: [51785-55-8].
$C_{14}H_{19}FO_9$ M 350.2 Syrup.

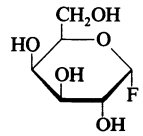
β-D-form

Tetra-Ac: [51785-54-7].
Cryst. (Et_2O/pentane). Mp 76-77°. $[\alpha]_D^{24}$ −15.2 (c, 1.5 in $CHCl_3$).

Tetrabenzoyl: [51785-56-9].
$C_{34}H_{27}FO_9$ M 598.5 Cryst. Mp 110-111°. $[\alpha]_D^{24}$ +14.9 (c, 1.6 in $CHCl_3$).

Bock, K. *et al, Acta Chem. Scand.*, 1973, **27**, 3586 (*α-tetra-Ac, β-tetra-Ac, β-tetrabenzoyl, pmr, F-19 nmr*)
Voznyi, Y.V. *et al, Bioorg. Khim.*, 1986, **12**, 521; *Sov. J. Bioorg. Chem. (Engl. Transl.)*, 1986, **12**, 277 (*β-tetra-Ac*)

Galactopyranosyl fluoride G-1-00003



α-D-*form*

$C_6H_{11}FO_5$ M 182.1

α-D-form

Tetra-Ac: [4163-44-4].
$C_{14}H_{19}FO_9$ M 350.2 Cryst. (Et_2O/heptane). Mp 67-68°. $[\alpha]_D^{25}$ +106.6 (c, 0.84 in $CHCl_3$).

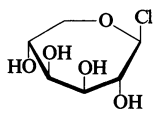
Tetrabenzyl: [94898-43-8].
$C_{34}H_{35}FO_5$ M 542.6 Syrup.

β-D-form

Tetra-Ac: [4163-45-5].
Cryst. (Et_2O). Mp 103-104° (98-99°). $[\alpha]_D^{18}$ +22 ($CHCl_3$).

Hall, L.D. *et al, Can. J. Chem.*, 1969, **47**, 1 (*tetra-Ac, pmr, F-19 nmr*)
Bock, K. *et al, Acta Chem. Scand., Ser. B*, 1975, **29**, 682 (*cmr, F-19 nmr*)
Voznij, Y.V. *et al, Carbohydr. Res.*, 1984, **132**, 339 (*tetra-Ac*)
Ger. Pat., 3 528 654, (1987); *CA*, **106**, 156814m (*tetra-Ac*)
Ger. Pat., 3 626 028, (1987); *CA*, **107**, 176407e (*tetra-Ac*)
Thiem, J. *et al, Synthesis*, 1988, 124 (*tetrabenzyl*)
Eur. Pat., 298 438, (1989); *CA*, **112**, 75339g (*synth*)

Galactoseptanosyl chloride G-1-00004



$C_6H_{11}ClO_5$ M 198.6

β-D-form

Syrup. $[\alpha]_D^{19}$ −79.5 ($CHCl_3$).

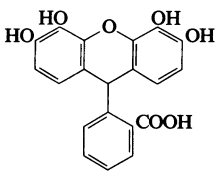
Tetra-Ac:
$C_{14}H_{19}ClO_9$ M 366.7 Cryst. (Et_2O). Mp 108°. $[\alpha]_D^{20}$ +170 (c, 1.0 in $CHCl_3$).

Micheel, F. *et al, Annalen*, 1933, **507**, 138 (*tetra-Ac*)

Gallin G-1-00005

2-(3,4,5,6-Tetrahydroxy-9H-xanthen-9-yl) benzoic acid, 9CI. 9-(2-Carboxyphenyl)-3,4,5,6-tetrahydroxyxanthene

[54750-05-9]



$C_{20}H_{14}O_7$ M 366.3
Triphenylmethane dye. Inhibitor of *Escherichia coli* ribonucleic acid polymerase.

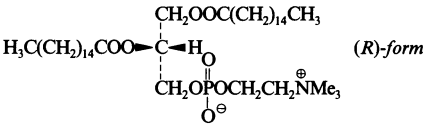
Liao, L.L. *et al, Biochemistry*, 1974, **13**, 1331.
Liao, L.-L. *et al, J. Med. Chem.*, 1975, **18**, 117.

Glycerol 1,2-dihexadecanoate 3-phosphocholine G-1-00006

Updated Entry replacing G-0-00393

Dipalmitoylphosphatidylcholine. 1,2-Dihexadecanoylglycero-3-phosphocholine. 1,2-Dipalmitoylglycero-3-phosphocholine. ***Colfosceril palmitate, BAN, INN, USAN.*** *Exosurf. Surfexo. Dipalmitoyllecithin*

[2644-64-6]



(*R*)-*form*

$C_{40}H_{80}NO_8P$ M 734.0
Surfactant. Launched 1994 (UK). Mixt. with 2-oleoyl-1-palmitoylglycero(3)phospho(1) glycerol also used (Pumactant, BAN), (ALEC).

(R)-form [63-89-8]
L-form. 129 Y83
Mp 235-236°. $[\alpha]_D^{25}$ +7.0 (c, 5.6 in $CHCl_3$).

[2797-68-4, 35418-55-4]

Baer, E. *et al, J.A.C.S.*, 1952, **74**, 158 (*synth*)
Brandt, A.E. *et al, Biochim. Biophys. Acta*, 1967, **144**, 605 (*synth*)
Vilallonga, F., *Biochim. Biophys. Acta*, 1968, **163**, 290 (*props*)
Saunders, D.R. *et al, Biochim. Biophys. Acta*, 1969, **176**, 828 (*props*)
Klein, R.A., *J. Lipid Res.*, 1971, **12**, 123 (*ms*)
Ghosh, D. *et al, Biochim. Biophys. Acta*, 1972, **266**, 41.
Birdsall, N.J.M. *et al, J.C.S. Perkin 2*, 1972, 1441 (*conformn, pmr, cmr*)
Gordon, D.T. *et al, Lipids*, 1972, **7**, 261 (*synth*)
Bunow, M.R. *et al, Biochim. Biophys. Acta*, 1977, **489**, 191 (*Raman*)
Urabe, T. *et al, Proc. Natl. Acad. Sci. U.S.A.*, 1981, **78**, 4941.
Regen, S.L. *et al, J.A.C.S.*, 1982, **104**, 791 (*synth*)
Hansen, W.J. *et al, Lipids*, 1982, **17**, 453 (*synth*)
Dekker, C.J. *et al, Chem. Phys. Lipids*, 1983, **33**, 93 (*synth, props*)
Lindh, I. *et al, J.O.C.*, 1989, **54**, 1338 (*synth*)
Dechant, K.L. *et al, Drugs*, 1991, **42**, 877 (*rev*)

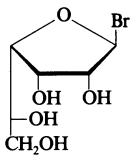
Glycol dimethacrylate G-1-00007

$H_2C{=}C(CH_3)COOCH_2CH_2OOCC(CH_3){=}CH_2$

$C_{10}H_{14}O_4$ M 198.2
Monomer. Liq. d 1.05. $Bp_{0.18}$ 58°. n_D^{20} 1.4549.

Walling, C., *J.A.C.S.*, 1945, **67**, 441.
Loshaek, S. *et al, J.A.C.S.*, 1953, **75**, 3544.

Gulofuranosyl bromide G-1-00008



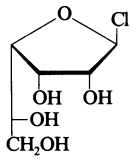
$C_6H_{11}BrO_5$ M 243.0

β-D-form

2,3:5,6-Di-O-(ethylboranediyl): [81975-74-8].
$C_{10}H_{17}B_2BrO_5$ M 318.7 Pale yellow syrup.

Dahlhoff, W.V. *et al*, *Heterocycles*, 1982, **18**, 421 (*deriv, ms, cmr, B-11 nmr*)

Gulofuranosyl chloride G-1-00009



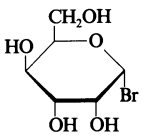
$C_6H_{11}ClO_5$ M 198.6

β-D-form

2,3:5,6-Di-O-isopropylidene: [16136-64-4].
$C_{12}H_{19}ClO_5$ M 278.7 Viscous oil. $Bp_{2.6}$ 127°. $[\alpha]_D^{25}$ −40.2 (c, 9.6 in $CHCl_3$).

Lerner, L.M. *et al*, *J.O.C.*, 1968, **33**, 1780 (*diisopropylidene, pmr*)

Gulopyranosyl bromide G-1-00010



α-D-*form*

$C_6H_{11}BrO_5$ M 243.0

α-D-form

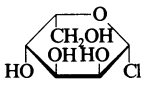
Tetra-Ac: [72002-90-5].
$C_{14}H_{19}BrO_9$ M 411.2 Syrup.

β-L-form

Tetra-Ac: [78418-57-2].
Syrup.

Shah, R.H. *et al*, *Carbohydr. Res.*, 1979, **74**, 105 (*α-tetra-Ac, reactions*)
Jacobsen, S. *et al*, *Acta Chem. Scand., Ser. B*, 1981, **35**, 163 (*α-tetra-Ac*)
Pozsgay, V. *et al*, *J.O.C.*, 1981, **46**, 3761 (*β-tetra-Ac*)

Gulopyranosyl chloride G-1-00011



$C_6H_{11}ClO_5$ M 198.6

β-L-form

3,4,6-Tribenzyl, 2-Ac: [78355-27-8].
$C_{29}H_{31}ClO_6$ M 511.0 Plates. Mp 79-80°. $[\alpha]_D^{25}$ +58.4 (c, 0.5 in $CHCl_3$).

Pozsgay, V. *et al*, *J.O.C.*, 1981, **46**, 3761 (*tribenzyl deriv*)
Katano, K. *et al*, *J.O.C.*, 1985, **50**, 5807 (*tribenzyl deriv, pmr*)

H

Hectane, 9CI H-1-00001

Decacontane

[6703-98-6]

$H_3C(CH_2)_{98}CH_3$

$C_{100}H_{202}$ M 1404.6

Longest defined hydrocarbon described at least up to 1973. Plates (butyl acetate). Mp 115.1-115.4°.

Ställberg, G. *et al, Acta Chem. Scand.*, 1952, **6**, 313 (*synth*)

1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9, 9,10,10,10-Heneicosafluorodecane, 8CI H-1-00002

1H-Perfluorodecane

[375-97-3]

$F_3C(CF_2)_8CF_2H$

$C_{10}HF_{21}$ M 520.0

Mp 31-33°. Bp 159-160°.

U.S. Pat., 2 490 764, (1949); *CA*, **44**, 3003g.

1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8, 9,9,10,10-Heneicosafluoro-10-iododecane H-1-00003

Perfluorodecyl iodide

[423-62-1]

$F_3C(CF_2)_8CF_2I$

$C_{10}F_{21}I$ M 645.9

Mp 65-67°. Bp 195-200°, Bp_{45} 102-106°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 130D.

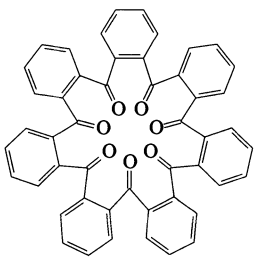
Haszeldine, R.N., *J.C.S.*, 1953, 3761 (*synth, uv*)

U.S. Pat., 3 404 189, (1968); *CA*, **70**, 11105 (*synth*)

***5H*-Heptabenzo[*a,d,g,j,m,p,s*]cycloheneicosene-5,10,15,20,25,30,35-heptone, 9CI** H-1-00004

[*l*$_7$]*Orthocyclophaneheptaone*

[154618-96-9]



$C_{49}H_{28}O_7$ M 728.7

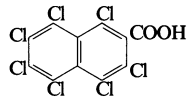
The nonaone ring system has also been prepd. Mp 252-253°.

Lee, W.Y. *et al, J.O.C.*, 1994, **59**, 878 (*synth, cryst struct, ir, pmr, cmr, ms*)

1,3,4,5,6,7,8-Heptachloro-2-naphthalenecarboxylic acid, 9CI H-1-00005

Perchloro-2-naphthoic acid

[163399-24-4]



$C_{11}HCl_7O_2$ M 413.2

Needles (Et_2O/hexane or by subl.). Mp 219-221°.

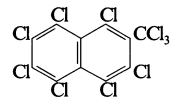
Me ester: [163399-25-5].
$C_{12}H_3Cl_7O_2$ M 427.3 Dimorphic cryst. (hexane). Mp 96-97° (prisms), Mp 116.5-117.5° (needles).

Carilla, J. *et al, J.O.C.*, 1995, **60**, 2721 (*synth, ir, uv, pmr, cmr*)

1,2,3,4,5,6,8-Heptachloro-7-(trichloromethyl)naphthalene, 9CI H-1-00006

Perchloro-2-methylnapthalene

[150986-19-9]



$C_{11}Cl_{10}$ M 486.6

Highly strained non-planar struct. Yellow prisms (hexane). Mp 119-120°.

Carilla, J. *et al, J.O.C.*, 1995, **60**, 2721 (*synth, ir, uv, cmr, cryst struct*)

1,18-Heptacosadiene H-1-00007

$H_3C(CH_2)_7CH{=}CH(CH_2)_{15}CH{=}CH_2$

$C_{27}H_{52}$ M 376.7

(E)-form [104899-45-8]
Isol. from the green alga *Botryococcus braunii.*

(Z)-form [104899-40-3]
Isol. from *B. braunii.*

Metzger, P. *et al, Phytochemistry*, 1986, **25**, 1869; 1993, **33**, 1125 (*isol, pmr, cmr*)

1,17-Heptadecanediol, 9CI H-1-00008

[66577-59-1]

$HOCH_2(CH_2)_{15}CH_2OH$

$C_{17}H_{36}O_2$ M 272.4

Occurs in leaf cutin of *Limonia acidissima.* Cryst. (C_6H_6). Mp 96-96.5° (93-94°). Bp_2 204-205°.

Chuit, P. *et al, Helv. Chim. Acta*, 1929, **12**, 850 (*synth*)

Percec, V. *et al, Macromolecules*, 1990, **23**, 3509 (*synth, pmr*)

Patwardhan, S.A., *Org. Prep. Proced. Int.*, 1994, **26**, 647 (*rev*)

2,4-Heptadecanedione, 9CI H-1-00009

[64042-18-8]

$H_3C(CH_2)_{12}COCH_2COCH_3$

$C_{17}H_{32}O_2$ M 268.4

Acetogenin. Constit. of *Ruta graveolens* and the alga *Caulocystis cephalornithos.* Also found in various mammalian tissues. Oil.

Douglas, D.E. *et al, Lipids*, 1977, **12**, 635 (*synth*)

Douglas, D.E. *et al, Can. J. Biochem.*, 1978, **56**, 691 (*occur*)

Tattje, D.H.E. *et al, Pharm. Weekbl.*, 1978, **113**, 1169 (*isol*)

Amico, V. *et al, J. Nat. Prod.*, 1990, **53**, 1379 (*isol*)

10-Heptadecen-1-ol, 9CI H-1-00010

[129396-63-0]

$H_3C(CH_2)_5CH{=}CH(CH_2)_8CH_2OH$

$C_{17}H_{34}O$ M 254.4

(Z)-form [73010-83-0]
Oil. $Bp_{0.001}$ 100°.

Pfeifer, J. *et al, Annalen*, 1995, 131 (*synth, ir, pmr, cmr*)

16-Heptadecen-1-ol, 9CI H-1-00011

[59396-42-8]

$H_2C{=}CH(CH_2)_{14}CH_2OH$

$C_{17}H_{34}O$ M 254.4

Fluffy cryst. (hexane). Mp 32-33°, Mp 44.5-45.5°.

Kung, H.F. *et al, Nucl. Med. Biol.*, 1991, **18**, 215; *CA*, **114**, 243537g (*synth, pmr, ir, ms*)

Cloux, R. *et al, Synthesis*, 1993, 909 (*synth, ir, pmr, cmr, ms*)

2,2,3,3,4,4,4-Heptafluoro-1-butylamine H-1-00012

[374-99-2]

$F_3CCF_2CF_2CH_2NH_2$

$C_4H_4F_7N$ M 199.0

d 1.49. Bp 70-71°, Bp_{115} 24°. n_D^{20} 1.298.

Hydrochloride: [2794-75-4].
Mp 130-135° subl.

Ac:
$C_6H_6F_7NO$ M 241.1 Mp 51-52°.

UK Pat., 717 232, (1954); *CA*, **49**, 12531f.

Ellzey, S.E. *et al, J.O.C.*, 1965, **30**, 3945 (*synth*)

3,3,4,4,5,5,5-Heptafluoro-1-pentene, 9CI, 8CI H-1-00013

[355-08-8]

$F_3CCF_2CF_2CH{=}CH_2$

$C_5H_3F_7$ M 196.0

d 1.34. Bp 30-31°. n_D^{20} 1.2752.

Pierce, O.R. *et al, J.A.C.S.*, 1953, 75, 5618.

Tarrant, P. *et al, J.A.C.S.*, 1957, 79, 6536.

Durrell, W. *et al, J.O.C.*, 1960, 25, 1662.
Burton, D.J. *et al, J. Fluorine Chem.*, 1988, 38, 119.

2,2,3,3,4,4,4-Heptafluoro-1-phenyl-1-butanone H-1-00014

1-Benzoyl-1,1,2,2,3,3,3-heptafluoropropane

[559-91-1]

$PhCOCF_2CF_2CF_3$

$C_{10}H_5F_7O$ M 274.1
Bp_{740} 173-174°. n_D^{20} 1.4130.

2,4-Dinitrophenylhydrazone: Mp 86-87°.
Semicarbazone: Mp 133-135°.

Simons, J.H. *et al, J.A.C.S.*, 1953, **75**, 5621.
McBee, E.T., *J.A.C.S.*, 1955, **77**, 917.
Dishart, K.T., *J.A.C.S.*, 1956, **78**, 2268 (***synth***)
Griffin, C.E., *Spectrochim. Acta*, 1960, **16**, 1464 (*ir*)

1,1,1,2,3,3,3-Heptafluoropropane, 9CI H-1-00015

Apaflurane, INN

[431-89-0]

$F_3CCHFCF_3$

C_3HF_7 M 170.0
Diagnostic agent. Used as a propellant in pharmaceutical aerosol sprays. Gas. Bp −8° to −7°.

Aldrich, P.E. *et al, J.O.C.*, 1963, **28**, 184 (*synth*)
Andreades, S., *J.A.C.S.*, 1964, **86**, 2003 (*synth, F-19 nmr*)
Naae, D.G. *et al, Org. Mass Spectrom.*, 1974, **9**, 1203 (*ms*)
Salvi-Narkhede, M. *et al, J. Chem. Thermodyn.*, 1992, **24**, 1065 (*props*)
Pat. Coop. Treaty (*WIPO*), 93 11 743, (1993) (*Glaxo*); *CA*, **119**, 80264c (*use*)

3-Hepten-1-yne, 9CI H-1-00016

[2806-40-8]

$H_3CCH_2CH_2CH{=}CHC{\equiv}CH$

C_7H_{10} M 94.1

(***E*)-*form*** [764-58-9]
Liq. Bp 107°, Bp_{164} 64.3°. n_D^{20} 1.4493.

(***Z*)-*form*** [764-57-8]
Liq. Bp 100-101°, Bp_{251} 66.2-66.3°. n_D^{20} 1.4437.

Butenandt, A. *et al, Annalen*, 1962, **658**, 39 (*synth, uv, ir*)
Montijn, P.P. *et al, Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1964, **83**, 456 (*synth, ir*)
Hearn, *J. Magn. Reson.*, 1976, **22**, 521 (*cmr*)
Carpita, A. *et al, Synth. Commun.*, 1994, **24**, 2281 (*synth, pmr*)

4-Hepten-6-yn-1-ol H-1-00017

[134225-67-5]

$HC{\equiv}CCH{=}CHCH_2CH_2CH_2OH$

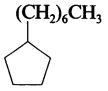
$C_7H_{10}O$ M 110.1
Incorr. called 4-en-5-yne in the ref. (*Z*)-form prepd. $Bp_{0.05}$ 68°. Bp refers to a mixture of isomers.

[135511-16-9, 135511-17-0]

Klusener, P.A.A. *et al, J. Organomet. Chem.*, 1991, **409**, 67.
Crombie, L. *et al, J.C.S. Perkin 1*, 1994, 673 (*synth, uv, pmr*)

Heptylcyclopentane H-1-00018

1-Cyclopentylheptane



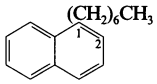
$C_{12}H_{24}$ M 168.3
d^{20} 0.801. Fp −53°. Bp 224°, Bp_{10} 95°. n_D^{20} 1.4421.

Adv. Chem. Ser., 1955, **15**, 385 (***props***)

1-Heptylnaphthalene H-1-00019

1-(1-Naphthalenyl)heptane

[2876-52-0]



$C_{17}H_{22}$ M 226.3
Liq. d^{20} 0.949. Fp −8°. Bp 340°, Bp_1 133-139°. n_D^{20} 1.5582.

Adv. Chem. Ser., 1955, **15**, 226 (***props***)

2-Heptylnapthalene H-1-00020

1-(2-Naphthalenyl)heptane

[2876-45-1]

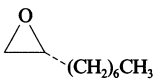
$C_{17}H_{22}$ M 226.3
d^{20} 0.941. Fp 1°. Bp 341°, Bp_1 134.6°. n_D^{20} 1.5556.

Adv. Chem. Ser., 1955, **15**, 227 (***props***)

Heptyloxirane, 9CI H-1-00021

1,2-Epoxynonane, 8CI

[2984-50-1]



(*R*)-*form*

$C_9H_{18}O$ M 142.2

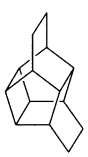
(***R*)-*form*** [130466-96-5]
Liq. Bp_{15} 76-78°. $[\alpha]_D^{20}$ +8.1 (c, 1 in $CHCl_3$) (96% ee).

(***S*)-*form*** [109856-84-0]
Liq. Bp_{15} 77-79°. $[\alpha]_D^{20}$ −8.6 (c, 1 in $CHCl_3$) (97% ee).

(±)-***form*** [152517-46-9]
Liq. Bp_{13} 75°. n_D^{20} 1.4235.

Rothstein, B., *Bull. Soc. Chim. Fr.*, 1935, **2**, 1936 (*synth*)
George, D.A. *et al, J. Chem. Eng. Data*, 1975, **20**, 445 (*ms*)
Sadhu, K.M. *et al, Tet. Lett.*, 1986, **27**, 795 (*synth, cmr*)
Haase, B. *et al, Tetrahedron: Asymmetry*, 1993, **4**, 1017 (*asymm synth*)
Müller, C. *et al, Annalen*, 1995, 677 (*synth*)

Hexacyclo [6.4.2.0^{2,7}.0^{3,11}.0^{6,10}.0^{9,12}] tetradecane H-1-00022



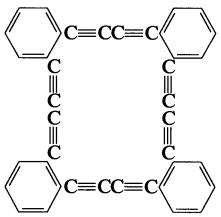
$C_{14}H_{18}$ M 186.2
Cryst. Mp 91-92°.

Takeshita, H. *et al, J.O.C.*, 1994, **59**, 6490 (*synth, pmr, cmr, ms, ir*)

5,6,7,8,13,14,15,16,21,23,24,29,30,31,32-Hexadecadehydrotetrabenzo [*a,g,m,s*]cyclotetracosene, 9CI H-1-00023

1,2:7,8:13,14:19,20-Tetrabenzocyclotetracosa-1,7,13,19-tetraene-3,5,9,11,15,17,21,23-octayne

[155587-92-1]



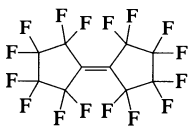
$C_{40}H_{16}$ M 496.5
Cryst.

Guo, L. *et al, Chem. Comm.*, 1994, 243 (*synth, cryst struct, pmr, cmr*)

Hexadecafluorobicyclopentylidene H-1-00024

Octafluoro(octafluorocyclopentylidene) cyclopentane, 9CI. Perfluorobicyclopentylidene

[49851-76-5]



$C_{10}F_{16}$ M 424.0
Bp 127°.

Chambers, R.D. *et al, J.C.S. Perkin 1*, 1973, 1710.
Smart, B.E. *et al, J.A.C.S.*, 1986, **108**, 4905.

Hexadecafluorodecanedioic acid H-1-00025

Perfluorosebacic acid

[307-78-8]

$HOOC(CF_2)_8COOH$

$C_{10}H_2F_{16}O_4$ M 490.0
Mp 160-161°.

Di-Me ester: [4590-24-3].
$C_{12}H_6F_{16}O_4$ M 518.1 Bp 261°.

Di-Et ester: [423-91-6].
$C_{14}H_{10}F_{16}O_4$ M 546.2 Bp_5 118-120°.

Dichloride: [1766-23-0].
$C_{10}Cl_2F_{16}O_2$ M 526.9 Mp 29-30°. Bp_{23} 101-103°.

Diamide: [307-77-7].
$C_{10}H_4F_{16}N_2O_2$ M 488.1 Cryst. (EtOH). Mp 239-241°.

Dinitrile: [2342-09-8].
$C_{10}F_{16}N_2$ M 452.0 Bp 147-148°.

Knunyants, I.L. *et al, Izv. Akad. Nauk SSSR, Otd. Khim. Nauk*, 1961, 1462; *CA*, **56**, 302i; 1963, 190; *CA*, **58**, 10072d (*synth, derivs*)
Ward, R.B., *J.O.C.*, 1965, **30**, 3009 (*diamide*)

McLoughlin, V.C.R., *Tet. Lett.*, 1968, 4761 (*Di-Me ester*)
Robinson, I.M. *et al*, *Macromolecules*, 1983, **16**, 526 (*Di-Me ester, ms*)

15-Hexadecen-1-ol, 9CI H-1-00026

[88591-06-4]

$H_2C{=}CH(CH_2)_{13}CH_2OH$

$C_{16}H_{32}O$ M 240.4
Solid (hexane). Mp 37-38°.

Ac: [85359-73-5].
$C_{18}H_{34}O_2$ M 282.4 Liq. n_D^{20} 1.4558.

Cloux, R. *et al*, *Synthesis*, 1992, 409; 1993, 909 (*synth, Ac, ir, pmr, cmr, ms*)

Hexadecylphosphonic acid H-1-00027

1-Phosphonohexadecane. 1-Hexadecanephosphonic acid

[4721-17-9]

$H_3C(CH_2)_{15}P(O)(OH)_2$

$C_{16}H_{35}O_3P$ M 306.4
Solid. Mp 94.5-95.5°.

Dibutyl ester: Dibutyl hexadecylphosphonate
$C_{24}H_{51}O_3P$ M 418.6 Liq. d_4^{25} 0.91. Bp_2 226-228°. n_D^{25} 1.4481.

Di-Ph ester: Diphenyl hexadecylphosphonate
$C_{28}H_{43}O_3P$ M 458.6 Cryst. (pentane). Mp 49.5-51°. $Bp_{0.01}$ 215°.

Dichloride: [4708-00-3].
$C_{16}H_{33}Cl_2OP$ M 343.3 Solid or liq. Mp 20-21°. Bp_2 178-180°.

Kosolapoff, G.M., *J.A.C.S.*, 1945, **67**, 1180.
Laughton, R.C., *J.O.C.*, 1962, **27**, 3664 (*dibutyl ester*)
Feshchenko, N.G. *et al*, *Zh. Obshch. Khim.*, 1967, **37**, 473; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1967, **37**, 441 (*dichloride*)
Dietze, U., *J. Prakt. Chem.*, 1974, **316**, 293 (*ir*)

4,5-Hexadien-1-amine, 9CI H-1-00028

6-Amino-1,2-hexadiene

[166303-35-1]

$H_2C{=}C{=}CHCH_2CH_2CH_2NH_2$

$C_6H_{11}N$ M 97.1
Bp 95-100°.

Shaw, R.W. *et al*, *J.C.S. Perkin 1*, 1994, 3549 (*synth, pmr*)

1,1,1,6,6,6-Hexafluoro-2,5-bis(trifluoromethyl)-2,3,4-hexatriene H-1-00029

Tetrakis(trifluoromethyl)butatriene. Perfluorobutatriene

$(F_3C)_2C{=}C{=}C{=}C(CF_3)_2$

C_8F_{12} M 324.0

Warrener, R.N. *et al*, *Tet. Lett.*, 1976, 2639.

1,1,2,2,3,3-Hexafluoro-1,3-diphenylpropane, 8CI H-1-00030

1,1'-(1,1,2,2,3,3-Hexafluoro-1,3-propanediyl) bisbenzene, 9CI

[2647-96-3]

$PhCF_2CF_2CF_2Ph$

$C_{15}H_{10}F_6$ M 304.2
Liq. Bp_5 133°.

U.K. Pat., 1 156 912, (1969); *CA*, **71**, 80905c (*manuf*)
Cotter, J.L., *Org. Mass Spectrom.*, 1973, **7**, 11 (*ms*)
Brel, V.K. *et al*, *J.O.C.*, 1993, **58**, 6922 (*synth, pmr, F-19 nmr, ms*)

1,1,1,3,3,3-Hexafluoro-2-hydroxy-2-propanephosphonic acid H-1-00031

[(2,2,2-Trifluoro-1-hydroxy-1-trifluoromethyl) ethyl]phosphonic acid

[125240-11-1]

$(F_3C)_2C(OH)P(O)(OH)_2$

$C_3H_3F_6O_4P$ M 248.0
Cryst. + $4H_2O$. Mp 94°.

Di-Me ester: [27375-65-1]. *Dimethyl [(2,2,2-trifluoro-1-hydroxy-1-trifluoromethyl)ethyl] phosphonate*
$C_5H_7F_6O_4P$ M 276.0 Liq. $Bp_{0.2}$ 31°.

Bis(trimethylsilyl) ester: [125240-07-5]. *Bis(trimethylsilyl) [(2,2,2-trifluoro-1-hydroxy-1-trifluoromethyl)ethyl] phosphonate*
$C_9H_{19}F_6O_4PSi_2$ M 392.3 Solid. Mp 80°.

Heine, J. *et al*, *Chem.-Ztg.*, 1989, **113**, 186 (*synth, ir, ms, pmr, F-19 nmr, P-31 nmr*)

1,1,1,3,3,3-Hexafluoro-2-methyl-2-propanol, 9CI, 8CI H-1-00032

1,1-Bis(trifluoromethyl)ethanol. Hexafluoro-2-methylisopropanol

[1515-14-6]

$H_3CC(CF_3)_2OH$

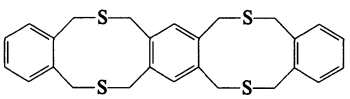
$C_4H_4F_6O$ M 182.0
Bp 60°. n_D^{20} 1.2970.

Trifluoroacetyl: [42031-16-3].
$C_6H_3F_9O_2$ M 278.0 Mp 65°.

Knunyants, I.L. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1961, 1471; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1961, 1370.
Howard, E.G. *et al*, *J.A.C.S.*, 1967, **89**, 1422 (*synth, F-19 nmr, pmr*)
Majid, A. *et al*, *J.O.C.*, 1973, **38**, 4028 (*deriv, synth, ms, ir, pmr, F-19 nmr*)
Walker, N. *et al*, *J. Magn. Reson.*, 1979, **34**, 295 (*cmr*)

5,9,11,16,20,22-Hexahydro-7*H*,18*H*-benzo[1,2-*d*:4,5-*d'*]bis[2,7]benzodithiecin H-1-00033

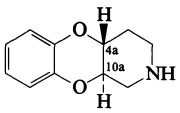
[159144-35-1]



$C_{26}H_{26}S_4$ M 466.7
Potential 2-coord. ligand. Mp >162°.

Hanton, L.R. *et al*, *J.C.S. Perkin 1*, 1994, 1883 (*synth, pmr*)

1,2,3,4,4*a*,10*a*-Hexahydro[1,4]benzodioxino[2,3-*c*]pyridine H-1-00034

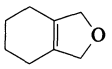


$C_{11}H_{13}NO_2$ M 191.2
A previously reported synth. (1970) was erroneous.

(4aRS,10aRS)-form
(±)-trans-*form*
Cryst. (MeOH) (as hydrochloride). Mp 272-274° (hydrochloride).

Procopiou, P.A. *et al*, *J.C.S. Perkin 1*, 1994, 1773.

1,3,4,5,6,7-Hexahydrobenzo[*c*]furan H-1-00035

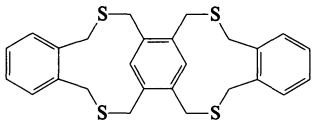


$C_8H_{12}O$ M 124.1
Liq. Bp_{15} 150°.

Brown, D.S. *et al*, *J.C.S. Perkin 1*, 1995, 1137 (*synth, ir, pmr, cmr, ms*)

5,7,10,12,17,24-Hexahydro-19*H*,22*H*-8,21:9,20-dimethenodibenzo[*c*,*m*][1,6,11,16]tetrathiacycloeicosin H-1-00036

[159144-34-0]



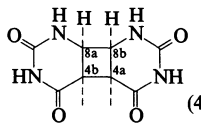
$C_{26}H_{26}S_4$ M 466.7
Cryst. (CH_2Cl_2/hexane). Mp >298° dec.

Hanton, L.R. *et al*, *J.C.S. Perkin 1*, 1994, 1883 (*synth, pmr, cryst struct*)

Hexahydro-4*a*,4*b*-dimethylcyclobuta[1,2-*d*:4,3-*d'*]dipyrimidine-2,4,5,7(3*H*,6*H*)-tetrone, 9CI H-1-00037

Thymine dimer. Thymine photodimer

[14122-25-9]



(4aα,4bα,8aα,8bα)-*form*

$C_{10}H_{12}N_4O_4$ M 252.2

(4aα,4bα,8aα,8bα)-form
cis-syn-*form*
Major product formed on uv irradn. of Thymine, T-0-03451. Needles (H_2O). Mp >300°.

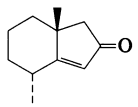
(4aα,4bβ,8aβ,8bα)-form [16452-84-9]
trans-syn-*form*
Minor prod. formed on uv irradn. of Thymine, T-0-03451. Cryst. (H_2O).

[13526-50-6]

Wulff, D.L. *et al*, *Biochim. Biophys. Acta*, 1961, **51**, 332 (*synth*)
Weinblum, D. *et al*, *Biochim. Biophys. Acta*, 1966, **114**, 450 (*synth*)
Jennings, B.H. *et al*, *Photochem. Photobiol.*, 1970, **11**, 215 (*synth, ir, ms, pmr*)
Wei, C.H. *et al*, *Acta Cryst. B*, 1984, **40**, 271 (*cryst struct*)

1,4,5,6,7,7*a*-Hexahydro-4,7*a*-dimethyl-2*H*-inden-2-one, 9CI H-1-00038

[65969-87-1]



(4*RS*,7*aRS*)-*form*

$C_{11}H_{16}O$ M 164.2

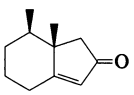
(4RS,7aRS)-form [76803-50-4]
(±)-trans-*form*
Oil. $Bp_{0.7}$ 78-80°.

(4RS,7aSR)-form [123992-65-4]
cis-*form*
Oil.

[52528-82-2, 130530-08-4]

Tokorayama, T. *et al*, *J.C.S. Perkin 1*, 1988, 445 (*synth, uv, pmr, ir*)
Ceccherelli, P. *et al*, *J.O.C.*, 1990, **55**, 311 (*synth, pmr, cmr*)
Weyerstahl, P. *et al*, *Annalen*, 1995, 191 (*synth, pmr, cmr, ms*)

1,4,5,6,7,7*a*-Hexahydro-7,7*a*-dimethyl-2*H*-inden-2-one, 9CI H-1-00039



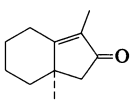
$C_{11}H_{16}O$ M 164.2

(7R,7aS)-form [39900-31-7]
Oil.

Evans, D.A. *et al*, *J.A.C.S.*, 1977, **99**, 5453 (*synth, pmr*)
Smith, A.B. *et al*, *J.A.C.S.*, 1981, **103**, 1996 (*synth, ir, pmr*)

3,3*a*,4,5,6,7-Hexahydro-1,3*a*-dimethyl-2*H*-inden-2-one, 9CI H-1-00040

[60415-97-6]



(*R*)-*form*

$C_{11}H_{16}O$ M 164.2

(R)-form [115692-65-4]
$[\alpha]_D^{25}$ −12 (c, 0.3 in EtOH).

(±)-form
$Bp_{0.2}$ 88-89°.

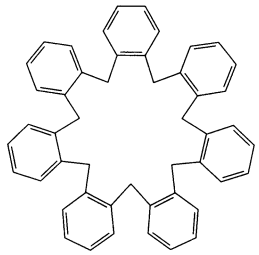
2,4-Dinitrophenylhydrazone: [127939-08-6]. Mp 203°.

Miyashita, M. *et al*, *J.A.C.S.*, 1984, **106**, 2149 (*synth, ir, pmr*)
Grattan, T.J. *et al*, *J.C.S. Perkin 1*, 1990, 11 (*synth, ms, ir, pmr*)

10,15,20,25,30,35-Hexahydro-5*H*-heptabenzo[*a,d,g,j,m,p,s*]cycloheneicosene, 9CI H-1-00041

[*1*$_7$]*Orthocyclophane*

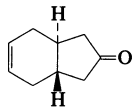
[154618-91-4]



$C_{49}H_{42}$ M 630.8
Powder. Mp 207-208°.

Lee, W.Y. *et al*, *J.O.C.*, 1994, **59**, 878 (*synth, ir, pmr, cmr, ms*)

1,3,3*a*,4,7,7*a*-Hexahydro-2*H*-inden-2-one H-1-00042



(3*aS*,7*aS*)-*form*

$C_9H_{12}O$ M 136.1

(3aS,7aS)-form
(+)-trans-*form*
Needles. Mp 66-67°. $[\alpha]_D$ +105.0 (c, 1.13 in EtOH).

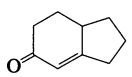
(3aRS,7aSR)-form
cis-*form*
Oil. Bp_{10} 106-108°.

Aubé, J. *et al*, *J.A.C.S.*, 1994, **116**, 9009 (*synth, pmr, cmr*)

1,2,3,6,7,7*a*-Hexahydro-5*H*-inden-5-one H-1-00043

Bicyclo[*4.3.0*]*non-1-en-3-one*

[1489-28-7]



$C_9H_{12}O$ M 136.1

(±)-*form* [119971-92-5]
Liq. Bp_{12} 107-112°, $Bp_{0.3}$ 75°.

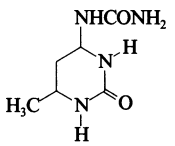
Semicarbazone: Cryst. (butanol). Mp 220°.

Prelog, V. *et al*, *Helv. Chim. Acta*, 1949, **32**, 2360 (*synth*)
Stork, G. *et al*, *J.A.C.S.*, 1963, **85**, 207 (*synth*)
Hollingworth, G.J. *et al*, *Aust. J. Chem.*, 1995, **48**, 381 (*synth, uv, pmr, cmr, bibl*)

(Hexahydro-6-methyl-2-oxo-4-pyrimidinyl)urea, 9CI, 8CI H-1-00044

Cyclodiurea

[1129-42-6]



$C_6H_{12}N_4O_2$ M 172.1

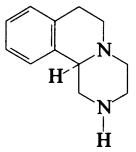
Fertiliser, feed additive for sheep. Rods (H_2O). Mp 245°.

Zigeuner, G. *et al*, *Monatsh. Chem.*, 1961, **92**, 31, 278 (*synth*)
Inoue, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 1915 (*synth*)

1,3,4,6,7,11*b*-Hexahydro-2*H*-pyrazino[2,1-*a*]isoquinoline, 9CI H-1-00045

Azaquinzole, INN

[5234-86-6]



(*R*)-*form*

$C_{12}H_{16}N_2$ M 188.2
CNS depressant. Never marketed.

(R)-form [99780-88-8]
$[\alpha]_D^{21}$ −140.3 (c, 0.56 in Py).

(±)-form
$Bp_{0.01}$ 98-100°.

Hydrochloride (1:2): Mp 320°.

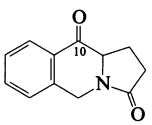
[99780-87-7]

Belg. Pat., 659 249, (1965) (*E Merck*); *CA*, **64**, 2107e (*synth, pharmacol*)
Ripperger, H. *et al*, *Chem. Ber.*, 1967, **100**, 1383 (*cd*)
Blaschke, G. *et al*, *Chem. Ber.*, 1985, **118**, 4620 (*isomers, cd, pmr*)
Jin, L. *et al*, *Yaoxue Xuebao*, 1986, **21**, 170; *CA*, **106**, 4976c (*sar*)

1,2,3,5,10,10*a*-Hexahydropyrrolo[1,2-*b*]isoquinoline-3,10-dione, 9CI H-1-00046

*1,2,3,5,10,10*a*-Hexahydrobenz*[f]*indolizine-3,10-dione*

[87630-51-1]



$C_{12}H_{11}NO_2$ M 201.2

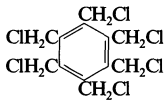
(±)-*form* [103201-08-7]
Yellow solid. Mp 107-108°.

10-Oxime (Z-)*:* [103201-11-2].
$C_{12}H_{12}N_2O_2$ M 216.2 Cryst. (95% EtOH aq.). Mp 213.5-216°.

Rigo, B. *et al*, *J. Het. Chem.*, 1983, **20**, 893 (*synth, ir, pmr*)
Martin, L.L. *et al*, *J.O.C.*, 1986, **51**, 3697 (*synth, oxime*)
Kolocouris, A. *et al*, *J. Crystallogr. Spectrosc. Res.*, 1993, **23**, 663 (*cryst struct, pmr, cmr*)
Rigo, B. *et al*, *Synth. Commun.*, 1994, **24**, 2609 (*synth*)

Hexakis(chloromethyl) benzene, 9CI H-1-00047

[40205-81-0]



$C_{12}H_{12}Cl_6$ M 368.9
Prisms (dioxan or pentachloroethane). Mp 287.5° (282-285°).

Backer, H.J., *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1936, **55**, 591 (*synth*)
Henzelmann, E. *et al*, *An. Asoc. Quim. Argent.*, 1972, **60**, 467; *CA*, **78**, 57881c (*synth*)

Hexamethyltellurium, 9CI H-1-00048

[129896-34-0]

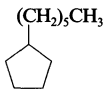
$TeMe_6$

$C_6H_{18}Te$ M 217.8
Volatile solid at −23°.

Ahmed, L. *et al*, *J.A.C.S.*, 1990, **112**, 7411.

Hexylcyclopentane H-1-00049

1-Cyclopentylhexane



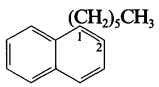
$C_{11}H_{22}$ M 154.2
d^{20} 0.800. Fp −73°. Bp 203°. n_D^{20} 1.4392.

Adv. Chem. Ser., 1955, **15**, 384 (***props***)

1-Hexylnaphthalene H-1-00050

1-(1-Naphthalenyl)hexane

[2876-53-1]



$C_{16}H_{20}$ M 212.3
Liq. d^{20} 0.957. Fp −18°. Bp 322°, Bp_1 121.4°. n_D^{20} 1.5647.

Adv. Chem. Ser., 1955, **15**, 224 (***props***)

2-Hexylnaphthalene H-1-00051

1-(2-Naphthalenyl)hexane

[2876-46-2]

$C_{16}H_{20}$ M 212.3
Liq. d^{20} 0.948. Fp −18°. Bp 324°, Bp_1 122.8°. n_D^{20} 1.5620.

Adv. Chem. Ser., 1955, **15**, 244 (***props***)
Dewprashad, B. *et al*, *Org. Prep. Proced. Int.*, 1989, **21**, 645 (*synth*)

Hexyl nitrate H-1-00052

[20633-11-8]

$H_3C(CH_2)_5ONO_2$

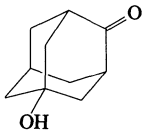
$C_6H_{13}NO_3$ M 147.1
Liq. $d_4^{24.5}$ 0.9745. Bp 171°, Bp_3 51-52°. n_D^{25} 1.4182.

Pattison, F.L.M. *et al*, *Can. J. Chem.*, 1956, **34**, 879 (*synth*)
Fraser, R.T.M. *et al*, *J.C.S.*(*B*), 1968, 659 (*ms*)
Olah, G.A. *et al*, *Synthesis*, 1993, 207 (*synth, cmr*)

5-Hydroxyadamantanone H-1-00053

5-Hydroxytricyclo[3.3.1.1^{3,7}]decan-2-one, 9CI.
Idramantone, INN. *Kemantane*

[20098-14-0]



$C_{10}H_{14}O_2$ M 166.2

(±)-form
Lymphocyte and antibody stimulant in mice, T-cell suppressor. Cryst. (CCl_4 or by subl.). Mp 319-322°.

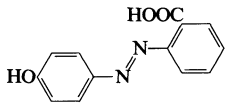
Ac: [63382-10-5].
$C_{12}H_{16}O_3$ M 208.2 Mp 60°.

Geluk, H.W. *et al*, *Tetrahedron*, 1968, **24**, 5369 (*synth, ir, pmr*)
Geluk, H.W., *Synthesis*, 1972, 374 (*synth*)
Vodicka, L. *et al*, *Coll. Czech. Chem. Comm.*, 1975, **40**, 293 (*pmr*)
Czech. Pat., 163 671, (1976); *CA*, **86**, 55081h (*synth*)
Lantvoev, V.I., *Zh. Org. Khim.*, 1976, **12**, 236; *J. Org. Chem. USSR* (*Engl. Transl.*), 1976, **12**, 2292 (*synth, ir*)
Morat, C. *et al*, *Tet. Lett.*, 1979, 4409 (*synth, Ac, ir, pmr, cmr*)
Le Noble, W.J. *et al*, *J.O.C.*, 1983, **48**, 1099 (*synth*)
Bolte, G. *et al*, *Chem. Ber.*, 1984, **117**, 1982 (*synth, pmr, ir, ms*)
Srivastava, S. *et al*, *Synth. Commun.*, 1984, **14**, 65 (*synth, bibl*)
Artsimovich, N.G. *et al*, *Immunologiya* (*Moscow*), 1990, **21**; *CA*, **114**, 156795w (*immunol*)
Boiko, S.S. *et al*, *CA*, 1991, **115**, 84695 (*glc*)

4′-Hydroxyazobenzene-2-carboxylic acid H-1-00054

2-[(4-Hydroxyphenyl)azo]benzoic acid, 9CI

[1634-82-8]



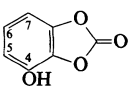
$C_{13}H_{10}N_2O_3$ M 242.2
Dye used in protein affinity binding studies, eg shows conc. dependent uv-vis shifts on binding to the biotin-complexing protein avidin. Light yellow-tan needles (MeOH). Mp 207-208°.

Ospenson, J.A. *et al*, *Acta Chem. Scand.*, 1951, **4**, 1351 (*synth*)
Harlow, R.L. *et al*, *Acta Cryst. C*, 1992, **48**, 48 (*cryst struct*)
Weber, P.C. *et al*, *J.A.C.S.*, 1994, **116**, 2717 (*use*)

4-Hydroxy-1,3-benzodioxol-2-one, 9CI H-1-00055

Pyrogallol carbonate

[6249-25-8]



$C_7H_4O_4$ M 152.1
Cryst. (C_6H_6). Mp 132-133°.

Einhorn, A. *et al*, *Ber.*, 1904, **37**, 100 (*synth*)

5-Hydroxy-1,3-benzodioxol-2-one, 9CI H-1-00056

[78213-00-0]

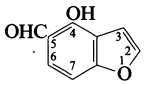
$C_7H_4O_4$ M 152.1
Cryst. (C_6H_6). Mp 176-178°.

Bredereck, H. *et al*, *Chem. Ber.*, 1958, **91**, 1314 (*synth*)

4-Hydroxy-5-benzofurancarboxaldehyde, 9CI H-1-00057

5-Formyl-4-hydroxybenzofuran

[59292-71-6]



$C_9H_6O_3$ M 162.1
Leaflets. Mp 58.5°.

Cagniant, P. *et al*, *C. R. Hebd. Seances Acad. Sci. Ser. C*, 1976, **282**, 465 (*synth*)
Lee, Y.R., *Tetrahedron*, 1995, **51**, 3087 (*synth, ir, pmr, cmr, ms*)

4-Hydroxy-7-benzofurancarboxaldehyde, 9CI H-1-00058

7-Formyl-4-hydroxybenzofuran

[59254-29-4]

$C_9H_6O_3$ M 162.1
Oil. Bp 168°.

René, L. *et al*, *Bull. Soc. Chim. Fr.*, 1975, 2763 (*synth*)

5-Hydroxy-4-benzofurancarboxaldehyde, 9CI H-1-00059

4-Formyl-5-hydroxybenzofuran

[59254-30-7]

$C_9H_6O_3$ M 162.1
Cryst. Mp 83°. Bp_{10} 141°.

René, L. *et al*, *Bull. Soc. Chim. Fr.*, 1975, 2763 (*synth*)

5-Hydroxy-6-benzofurancarboxaldehyde, 9CI H-1-00060

6-Formyl-5-hydroxybenzofuran

[63376-65-8]

$C_9H_6O_3$ M 162.1
Cryst. (EtOAc/hexane). Mp 114-115°.

Hammond, M.L. *et al*, *J. Med. Chem.*, 1990, **33**, 908 (*synth, pmr*)

6-Hydroxy-5-benzofurancarboxaldehyde, 9CI H-1-00061

5-Formyl-6-hydroxybenzofuran

[20073-22-7]

$C_9H_6O_3$ M 162.1
Needles (petrol). Mp 106.5-107.5°.

Me ether: [20073-21-6]. *6-Methoxy-5-benzofurancarboxaldehyde*

$C_{10}H_8O_3$ M 176.1 Cryst. (cyclohexane). Mp 88.5-90°.

Worden, L.R. *et al*, *J.O.C.*, 1969, **34**, 2311 (*synth, pmr*)

6-Hydroxy-7-benzofurancarboxaldehyde, 9CI H-1-00062

7-Formyl-6-hydroxybenzofuran

[59254-31-8]

$C_9H_6O_3$ M 162.1
Cryst. Mp 90°. Bp_{11} 130°.

René, L. *et al*, *Bull. Soc. Chim. Fr.*, 1975, 2763 (*synth*)

7-Hydroxy-4-benzofurancarboxaldehyde H-1-00063

4-Formyl-7-hydroxybenzofuran

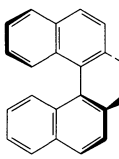
[6126-64-3]

$C_9H_6O_3$ M 162.1
Oil. Bp 191°.

René, L. *et al*, *Bull. Soc. Chim. Fr.*, 1975, 2763 (*synth*)

(2′-Hydroxy[1,1′-binaphthalen]-2-yl)diphenylphosphine H-1-00064

2-Hydroxy-2′-(diphenylphosphinyl)-1,1′-binaphthyl



(*S*)-*form*

$C_{32}H_{23}OP$ M 454.5
Widely appl. as catalyst in asymmetric reductions and hydrosilylations.

(S)-form

$[\alpha]_D^{20}$ −5.01 (c, 0.45 in $CHCl_3$).

Me ether: [134484-36-9]. *2-Methoxy-2′-(diphenylphosphinyl)-1,1′-binaphthyl*
$C_{33}H_{25}OP$ M 468.5 Cryst. (CH_2Cl_2/hexane). $[\alpha]_D^{20}$ −94.5 (c, 0.27 in $CHCl_3$), $[\alpha]_D^{20}$ −59.7 (c, 1.40 in C_6H_6).

Isopropyl ether: [137769-30-3].
$C_{35}H_{29}OP$ M 496.5 $[\alpha]_D^{20}$ −90.0 (c, 0.13 in $CHCl_3$).

Benzyl ether:
$C_{39}H_{29}OP$ M 544.6 $[\alpha]_D^{20}$ −96.1 (c, 0.12 in $CHCl_3$).

O-tert-*Butyldimethylsilyl:*
$C_{38}H_{37}OPSi$ M 568.7 $[\alpha]_D^{20}$ +29.3 (c, 0.71 in $CHCl_3$).

Oxide:
$C_{32}H_{23}O_2P$ M 470.5 $[\alpha]_D^{20}$ +105.0 (c, 0.52 in $CHCl_3$).

Oxide, O-*trifluoromethanesulfonyl:*
$C_{33}H_{22}F_3O_4PS$ M 602.5 $[\alpha]_D^{20}$ −44.45 (c, 0.50 in $CHCl_3$), $[\alpha]_D^{20}$ −6.61 (c, 1.40 in $CHCl_3$). Optical rotation v. dependent on concn.

Oxide, Me ether: [134484-37-0].
$C_{33}H_{25}O_2P$ M 484.5 $[\alpha]_D^{20}$ −126.9 (c, 0.52 in $CHCl_3$).

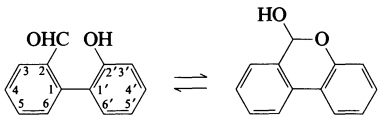
Oxide, isopropyl ether: [137769-27-8].
$C_{35}H_{29}O_2P$ M 512.5 $[\alpha]_D^{20}$ −315.2 (c, 0.13 in $CHCl_3$).

Oxide, benzyl ether:
$C_{39}H_{29}O_2P$ M 560.6 $[\alpha]_D^{20}$ −116.5 (c, 0.11 in $CHCl_3$).

Hayashi, T. *et al*, *Pure Appl. Chem.*, 1992, **64**, 1911 (*use*)
Matsumoto, Y. *et al*, *Chem. Comm.*, 1993, 1468 (*use*)
Uozumi, Y. *et al*, *J.O.C.*, 1993, **58**, 1945 (*synth, derivs, ir, ms, pmr, P-31 nmr*)
Uozumi, Y. *et al*, *Tetrahedron: Asymmetry*, 1993, **4**, 2419 (*use*)
Uemura, M. *et al*, *J. Organomet. Chem.*, 1994, **473**, 129 (*use*)
Matsumoto, H. *et al*, *J.A.C.S.*, 1994, **116**, 775 (*use*)

2′-Hydroxy-2-biphenylcarboxaldehyde H-1-00065

2-Formyl-2′-hydroxybiphenyl. 6H-Dibenzo[b,d]*pyran-6-ol*



$C_{13}H_{10}O_2$ M 198.2
Exists in the cyclic form. Obt. by oxidn. of Fluorene, F-0-00134.

Oxo-form [67608-60-0]

Me ether: [93465-26-0]. *2-Methoxy-2-biphenylcarboxaldehyde*
$C_{14}H_{12}O_2$ M 212.2 Cryst. (pentane). Mp 63-65°.

Cyclic-form [83358-32-1]

Me ether: 6-Methoxy-6H-dibenzo[b,d]*pyran*
$C_{14}H_{12}O_2$ M 212.2 Cryst. (pentane). Mp 56-70°.

Narasimhan, S. *et al*, *Indian J. Chem., Sect. B*, 1978, **16**, 516 (*synth, ms*)
Bonzatti, C. *et al*, *Arzneim.-Forsch.*, 1984, **34**, 864 (*synth*)
Bonzatti, C. *et al*, *Indian J. Chem., Sect. B*, 1984, **23**, 671 (*synth, ir, pmr, ms*)

3-Hydroxy-4-biphenylcarboxaldehyde, 9CI H-1-00066

4-Formyl-3-hydroxybiphenyl

[35664-67-6]

$C_{13}H_{10}O_2$ M 198.2
Cryst. (petrol). Mp 82-83°.

Spagnolo, P. *et al*, *J.C.S. Perkin 1*, 1972, 556 (*synth*)

4-Hydroxy-3-biphenylcarboxaldehyde H-1-00067

3-Formyl-4-hydroxybiphenyl

[1761-63-3]

$C_{13}H_{10}O_2$ M 198.2
Pale yellow plates (EtOH). Mp 102°.

Bell, F. *et al*, *J.C.S.*, 1926, 3047 (*synth*)
Duff, J.C., *J.C.S.*, 1941, 547 (*synth*)

4′-Hydroxy-4-biphenylcarboxaldehyde, 9CI H-1-00068

4-Formyl-4′-hydroxybiphenyl

[100980-82-3]

$C_{13}H_{10}O_2$ M 198.2
Cryst. Mp 178°.

Lourak, M. *et al*, *J.O.C.*, 1989, **54**, 4844 (*synth, ir, pmr*)

6-Hydroxy-3-biphenylcarboxaldehyde H-1-00069

5-Formyl-2-hydroxybiphenyl

[21363-10-0]

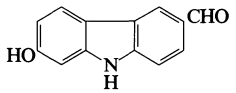
$C_{13}H_{10}O_2$ M 198.2
Cryst. (EtOH aq.). Mp 45-46°.

Jensen, S. *et al*, *Acta Chem. Scand.*, 1968, **22**, 2471 (*synth*)

7-Hydroxy-9*H*-carbazole-3-carboxaldehyde, 9CI H-1-00070

6-Formyl-2-hydroxycarbazole

[142750-13-8]

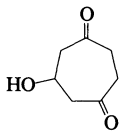


$C_{13}H_9NO_2$ M 211.2
Alkaloid from root bark of *Murraya euchrestifolia* (Rutaceae). Powder (Me_2CO).

Ito, C. *et al*, *Chem. Pharm. Bull.*, 1992, **40**, 230 (*isol, uv, ir, pmr, ms, struct*)

6-Hydroxy-1,4-cycloheptanedione H-1-00071

[150044-67-0]

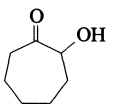


$C_7H_{10}O_3$ M 142.1
Isol. from *Pseudomonas* sp. AT3. Intermed. in bacterial degradn. of Tropine tropate, T-0-06922.

Bartholomew, B.A. *et al*, *Biochem. J.*, 1993, **293**, 115 (*isol*)

2-Hydroxycycloheptanone, 9CI H-1-00072

[4436-58-2]



$C_7H_{12}O_2$ M 128.1

(±)-form
Liq. Bp_{13} 91-94°.

Ac: [19347-07-0].
$C_9H_{14}O_3$ M 170.2 Liq. Bp_{10} 120-122°.

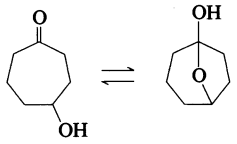
[154439-14-2]

Braun, M. *et al*, *Chem. Ber.*, 1976, **109**, 669 (*synth, ir, pmr*)
Reddy, G.S. *et al*, *Synthesis*, 1981, 223 (*synth, Ac*)
Moriarty, R.M. *et al*, *Tet. Lett.*, 1992, **33**, 6065 (*synth*)
Carnell, A.J. *et al*, *Tet. Lett.*, 1994, **35**, 331 (*synth*)

4-Hydroxycycloheptanone, 9CI H-1-00073

8-Oxabicyclo[3.2.1]octan-1-ol

[67963-12-6]



$C_7H_{12}O_2$ M 128.1

Exists as an equilib. mixt. of the keto and the hemiacetal forms.

(±)-*form*

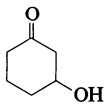
Liq. Bp_2 94°.

[151648-04-3]

Doering, W. von E. *et al*, *J.O.C.*, 1961, **26**, 1365 (*synth, ir*)
Suzuki, M. *et al*, *Heterocycles*, 1990, **30**, 517 (*synth, ir, pmr*)
Bäckvall, J.E. *et al*, *Tet. Lett.*, 1993, **34**, 5459 (*synth*)

3-Hydroxycyclohexanone, 9CI H-1-00074

[823-19-8]



$C_6H_{10}O_2$ M 114.1

(±)-*form*

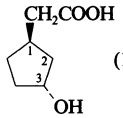
Liq. $Bp_{0.1}$ 80°.

[17429-00-4, 53164-77-5, 114764-49-7]

Molander, G.A. *et al*, *J.O.C.*, 1986, **51**, 2596 (*synth, ir, pmr, cmr*)
Miyashita, M. *et al*, *Tet. Lett.*, 1987, **28**, 4293 (*synth*)

3-Hydroxycyclopentaneacetic acid, 9CI H-1-00075

[102539-66-2]



(1*RS*,3*RS*)-*form*

$C_7H_{12}O_3$ M 144.1

***(1RS,3RS)*-form**

(±)-trans-*form*

Me ester: [138903-81-8].
$C_8H_{14}O_3$ M 158.1 Liq. $Bp_{0.5}$ 130°.

***(1RS,3SR)*-form**

(±)-cis-*form*

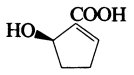
Me ester: [37435-80-6].
Bp_1 92-94°.

Lactone: [5724-61-8]. *2-Oxabicyclo[3.2.1]octan-3-one, 9CI*
$C_7H_{10}O_2$ M 126.1 Waxy cryst. Mp 58-59.5°.

[62358-07-0]

Barraclough, P. *et al*, *J.C.S. Perkin 1*, 1976, 264 (*synth, ester*)
House, H.O. *et al*, *J.O.C.*, 1983, **48**, 1693 (*synth, ir, pmr, cmr, ms, Me ester, lactone*)
Jenny, T.F. *et al*, *Helv. Chim. Acta*, 1992, **75**, 1944 (*synth, ir, pmr, cmr, ms, Me ester*)

5-Hydroxy-1-cyclopentene-1-carboxylic acid, 9CI H-1-00076



(*R*)-*form*

$C_6H_8O_3$ M 128.1

***(R)*-form**

Et ester: [143168-17-6].
$C_8H_{12}O_3$ M 156.1 Oil. $[\alpha]_D^{31}$ +34.4 (c, 1.0 in $CHCl_3$).

***(S)*-form**

Et ester: [143168-18-7].
Oil. Bp_1 45°. $[\alpha]_D^{31}$ −34.5 (c, 1.1 in $CHCl_3$).

(±)-*form*

Et ester: [115401-40-6].
Oil. $Bp_{0.06}$ 49-50°.

Nitrile: [130252-14-1]. *1-Cyano-5-hydroxy-1-cyclopentene*
C_6H_7NO M 109.1 Oil. $Bp_{0.1}$ 84-85°.

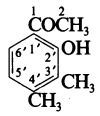
[86488-29-1, 106924-48-5]

Graff, M. *et al*, *Tet. Lett.*, 1986, **27**, 1577 (*synth, Et ester, nitrile*)
Takano, S. *et al*, *Tetrahedron: Asymmetry*, 1992, **3**, 837 (*asymm synth, Et ester*)
Yamane, T. *et al*, *Synthesis*, 1995, 444 (*synth, Et ester*)

2′-Hydroxy-3′,4′-dimethylacetophenone H-1-00077

1-(2-Hydroxy-3,4-dimethylphenyl)ethanone, 9CI

[5384-55-4]



$C_{10}H_{12}O_2$ M 164.2
Yellow oil. Bp_{12} 140°.

Semicarbazone: Cryst. (EtOAc). Mp 247° dec.

Me ether: 2′-Methoxy-3′,4′-dimethylacetophenone
$C_{11}H_{14}O_2$ M 178.2 Oil. Bp_2 104°.

v. Auwers, K. *et al*, *Annalen*, 1928, **460**, 240 (*synth*)
Smith, L.I. *et al*, *J.O.C.*, 1941, **6**, 427 (*synth*)
Baker, W. *et al*, *J.C.S.*, 1953, 1615 (*synth*)
Gardner, D. *et al*, *J.C.S.*, 1954, 1817 (*synth, Me ether*)

2′-Hydroxy-3′,5′-dimethylacetophenone H-1-00078

1-(2-Hydroxy-3,5-dimethylphenyl)ethanone, 9CI

[1198-66-9]

$C_{10}H_{12}O_2$ M 164.2
Pale yellow needles (EtOH aq.). Mp 54°. Bp_{16} 124.5-126°.

Oxime: [73170-30-6].
$C_{10}H_{13}NO_2$ M 179.2 Cryst. (petrol). Mp 140°.

Me ether: 2′-Methoxy-3′,5′-dimethylacetophenone
$C_{11}H_{14}O_2$ M 178.2 Needles (petrol). Mp 75-76°.

v. Auwers, K. *et al*, *Ber.*, 1925, **58**, 36 (*synth*)
Cocker, W. *et al*, *J.C.S.*, 1947, 533 (*Me ether*)
Trave, R., *Gazz. Chim. Ital.*, 1950, **80**, 502 (*synth, oxime*)
Cullinane, N.M. *et al*, *J. Appl. Chem.*, 1959, **9**, 133 (*synth*)
U.S. Pat., 3 900 521, (1975); *CA*, **83**, 205942u (*synth*)

2′-Hydroxy-4′,5′-dimethylacetophenone H-1-00079

1-(2-Hydroxy-4,5-dimethylphenyl)ethanone, 9CI

[36436-65-4]

$C_{10}H_{12}O_2$ M 164.2
Plates (petrol); needles (EtOH). Mp 71°.

Oxime:
$C_{10}H_{13}NO_2$ M 179.2 Cream cryst. (EtOH aq.). Mp 135.5°.

Semicarbazone: Leaflets (EtOH). Mp >275°.

Me ether: 2′-Methoxy-4′,5′-dimethylacetophenone
$C_{11}H_{14}O_2$ M 178.2 Prisms (petrol). Mp 55.5°.

Baddeley, G., *J.C.S.*, 1943, 273 (*synth*)
Baker, W. *et al*, *J.C.S.*, 1953, 820 (*synth*)
Royer, R. *et al*, *Bull. Soc. Chim. Fr.*, 1957, 1379 (*synth, oxime, Me ether*)
Vène, J. *et al*, *Bull. Soc. Chim. Fr.*, 1963, 1813 (*Me ether*)
Fischer, A. *et al*, *Can. J. Chem.*, 1975, **53**, 1570 (*synth, ir, pmr, ms*)
Burnell, R.H. *et al*, *Can. J. Chem.*, 1978, **56**, 517 (*synth, ir, uv, pmr*)

2′-Hydroxy-4′,6′-dimethylacetophenone H-1-00080

1-(2-Hydroxy-4,6-dimethylphenyl)ethanone, 9CI

[16108-50-2]

$C_{10}H_{12}O_2$ M 164.2
Pale yellow needles (petrol). Mp 60° (55-56°). Bp_{10} 130-132°.

Me ether: [21009-92-7]. *2′-Methoxy-4′,6′-dimethylacetophenone*
$C_{11}H_{14}O_2$ M 178.2 Cryst. (petrol). Mp 48°. Bp_{18} 140-144°.

v. Auwers, K., *Ber.*, 1915, **48**, 90 (*synth*)
Fuson, R.C. *et al*, *J.A.C.S.*, 1943, **65**, 1028 (*Me ether*)
Baddeley, G., *J.C.S.*, 1943, 273 (*synth*)
Edwards, J.D. *et al*, *J.A.C.S.*, 1956, **78**, 3821 (*Me ether*)
Bonsall, C. *et al*, *J.C.S.(C)*, 1967, 1836 (*pmr, uv*)
Ishido, Y. *et al*, *J.C.S. Perkin 1*, 1977, 521 (*synth, ir, pmr*)
Clark, J.H. *et al*, *J.C.S. Perkin 1*, 1977, 2063 (*synth, ms, ir*)

4-Hydroxy-2′,3′-dimethylacetophenone H-1-00081

1-(4-Hydroxy-2,3-dimethylphenyl)ethanone, 9CI

[5384-57-6]

$C_{10}H_{12}O_2$ M 164.2
Prisms (EtOH). Mp 145°.

Benzyl ester: [97888-86-3].
$C_{17}H_{18}O_2$ M 254.3 Cryst. (H_2O). Mp 85-86°.

Me ether: 4′-Methoxy-2′,3′-dimethylacetophenone
$C_{11}H_{14}O_2$ M 178.2 Plates (petrol). Mp 33°. Bp_{15} 157-159°.

Gardner, D. *et al*, *J.C.S.*, 1954, 1817 (*synth, Me ether*)
Vène, J. *et al*, *Bull. Soc. Chim. Fr.*, 1963, 1813 (*synth, Me ether*)

Royer, R. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 1259 (*synth, Me ether*)
Hajós, A., *Acta Chim. Hung.*, 1985, **118**, 63 (*synth, benzyl ether*)

4′-Hydroxy-2′,5′-dimethylacetophenone H-1-00082

1-(4-Hydroxy-2,5-dimethylphenyl)ethanone, 9CI

[26216-10-4]

$C_{10}H_{12}O_2$ M 164.2
Cryst. (toluene). Mp 131-132°.

Me ether: 4′-Methoxy-2′,5′-dimethylacetophenone
$C_{11}H_{14}O_2$ M 178.2 Plates (petrol). Mp 78-79°.

Clemo, G.R. *et al*, *J.C.S.*, 1929, 2368 (*Me ether*)
Kindler, K. *et al*, *Arch. Pharm. (Weinheim, Ger.)*, 1954, **287**, 210 (*synth*)

4′-Hydroxy-2′,6′-dimethylacetophenone H-1-00083

1-(4-Hydroxy-2,6-dimethylphenyl)ethanone, 9CI

[91060-92-3]

$C_{10}H_{12}O_2$ M 164.2

Me ether: [60999-76-0]. *4′-Methoxy-2′,6′-dimethylacetophenone*
$C_{11}H_{14}O_2$ M 178.2 Cryst. (EtOH). Mp 47°.

Laarhoven, W.H. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1961, **80**, 775.

4′-Hydroxy-3′,5′-dimethylacetophenone H-1-00084

1-(4-Hydroxy-3,5-dimethylphenyl)ethanone, 9CI

[5325-04-2]

$C_{10}H_{12}O_2$ M 164.2
Constit. of oil of *Eryngium foetidum*. Pale yellow plates (MeOH aq.). Mp 162° (154-155°).

Me ether: [60609-65-6]. *4′-Methoxy-3′,5′-dimethylacetophenone*
$C_{11}H_{14}O_2$ M 178.2 Cryst. (Et_2O). Mp 47-48° (39-40°).

Benington, F. *et al*, *J.O.C.*, 1958, **23**, 1979 (*synth, Me ether*)
Yeh, P.-H., *J. Chin. Chem. Soc. (Taipei)*, 1974, **22**, 139; *CA*, **82**, 34950t (*isol, ir, pmr*)
Eur. Pat., 609 885, (1994); *CA*, **121**, 255676j (*synth, pmr*)
Bhalerao, U.T. *et al*, *Synth. Commun.*, 1995, **25**, 1433 (*synth, pmr, ir*)

5′-Hydroxy-2′,4′-dimethylacetophenone H-1-00085

$C_{10}H_{12}O_2$ M 164.2
Needles (H_2O or EtOH). Mp 135° (130-131.5°).

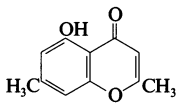
Me ether: 5′-Methoxy-2′,4′-dimethylacetophenone
$C_{11}H_{14}O_2$ M 178.2 Cryst. Mp 50-51°.

v. Auwers, K. *et al*, *Ber.*, 1928, **61**, 1495 (*synth, Me ether*)
Cullinane, N.M. *et al*, *J. Appl. Chem.*, 1959, **9**, 133 (*synth*)

5-Hydroxy-2,7-dimethyl-4*H*-1-benzopyran-4-one, 9CI H-1-00086

*5-Hydroxy-2,7-dimethylchromone. **Altechromone A***

[62806-16-0]

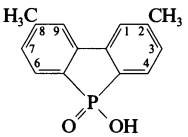


$C_{11}H_{10}O_3$ M 190.1
Prod. by *Alternaria* sp. Plant growth regulator. Needles + $\frac{1}{2}H_2O$ (C_6H_6/Me_2CO). Mp 251-252°.

Ahluwalia, V.K. *et al*, *Indian J. Chem., Sect. B*, 1976, **14**, 326 (*synth*)
Kimura, Y. *et al*, *Biosci., Biotechnol., Biochem.*, 1992, **56**, 1664 (*isol*)

5-Hydroxy-2,8-dimethyl-5*H*-dibenzophosphole 5-oxide H-1-00087

3,6-Dimethylphosphafluorenic acid



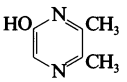
$C_{14}H_{13}O_2P$ M 244.2
Cryst. (EtOH aq.). Mp 303-305°.

Freedman, L.D. *et al*, *J.O.C.*, 1958, **24**, 638 (*synth, uv*)

5-Hydroxy-2,3-dimethylpyrazine H-1-00088

5,6-Dimethyl-2(1H)-pyrazinone, 9CI. 5,6-Dimethyl-2-pyrazinol

[57229-36-4]



$C_6H_8N_2O$ M 124.1
Cryst. Mp 201-202°.

Jones, R.G. *et al*, *J.A.C.S.*, 1949, **71**, 78 (*synth*)
Karmas, G. *et al*, *J.A.C.S.*, 1952, **74**, 1580 (*synth*)

5-Hydroxy-2,3-dimethylpyridine H-1-00089

5,6-Dimethyl-3-pyridinol, 9CI

[61893-00-3]

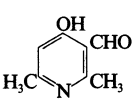
C_7H_9NO M 123.1
Solid (hexane/$CHCl_3$). Mp 147-149°.

Wai, J.S. *et al*, *J. Med. Chem.*, 1993, **36**, 249 (*synth, pmr*)

4-Hydroxy-2,6-dimethyl-3-pyridinecarboxaldehyde H-1-00090

1,4-Dihydro-2,6-dimethyl-4-oxo-3-pyridinecarboxaldehyde, 9CI. 3-Formyl-2,6-dimethyl-4(1H)-pyridinone

[138642-53-2]



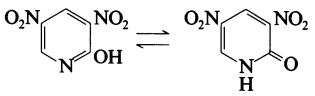
$C_8H_9NO_2$ M 151.1
Cryst. Mp >100° dec.

Bradbury, R.H. *et al*, *J. Med. Chem.*, 1993, **36**, 1245 (*synth, pmr*)

2-Hydroxy-3,5-dinitropyridine H-1-00091

3,5-Dinitro-2(1H)-pyridinone, 9CI. 3,5-Dinitro-2-pyridinol, 8CI

[2980-33-8]



$C_5H_3N_3O_5$ M 185.0
Yellow cryst. (AcOH). Mp 176-178° (168-170°).

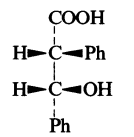
Me ether: [18617-40-8]. *2-Methoxy-3,5-dinitropyridine*
$C_6H_5N_3O_5$ M 199.1 Cryst. (EtOH aq.). Mp 92°.

Et ether: [18617-41-9]. *2-Ethoxy-3,5-dinitropyridine*
$C_7H_7N_3O_5$ M 213.1 Cryst. (EtOH aq.). Mp 71°.

Signor, A. *et al*, *Gazz. Chim. Ital.*, 1963, **93**, 65 (*synth*)
Matsumura, E. *et al*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 2413 (*synth*)
de Bie, D.A. *et al*, *J.O.C.*, 1985, **50**, 484 (*synth*)
Ritter, H. *et al*, *J. Het. Chem.*, 1995, **32**, 585 (*synth*)

3-Hydroxy-2,3-diphenylpropanoic acid H-1-00092

β-Hydroxy-α-phenylbenzenepropanoic acid



(*2RS,3RS*)-*form*

$C_{15}H_{14}O_3$ M 242.2

(2RS,3RS)-form
(±)-erythro-*form*
Mp 142-143.5°.

(2RS,3SR)-form
(±)-threo-*form*
Mp 177-178° (175°).

[4603-32-1, 4603-33-2, 58769-51-0, 93059-95-1]

Zimmerman, H.E. *et al*, *J.A.C.S.*, 1957, **79**, 1920 (*synth*)
Kolev, T. *et al*, *Acta Cryst. C*, 1995, **51**, 1169, 1350 (*cryst struct, dimethylamide, Me ester*)

2-Hydroxyethanesulfinic acid, 9CI H-1-00093

Isethinic acid

[60601-05-0]

$HOCH_2CH_2S(O)OH$

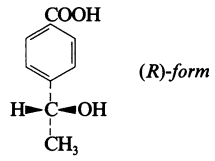
$C_2H_6O_3S$ M 110.1
Pale yellow oil.

Na salt: [43166-41-2].
Cryst. Mp 81-83°.

King, J.F. *et al*, *Can. J. Chem.*, 1983, **61**, 1583 (*synth, ir, pmr*)
Lee, C. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1990, **47**, 53 (*synth*)

4-(1-Hydroxyethyl)benzoic acid, 9CI H-1-00094

[97364-15-3]



(*R*)-form

$C_9H_{10}O_3$ M 166.1
Esters used as intermed. for liq. cryst.

(*R*)-form [125577-90-4]

Me ester: [129446-47-5].
$C_{10}H_{12}O_3$ M 180.2 Cryst. Mp 52-53°. $[\alpha]_D^{20}$ +42.3 (c, 1 in $CHCl_3$).

Et ester: [128310-70-3].
$C_{11}H_{14}O_3$ M 194.2 Liq. $[\alpha]_D^{21}$ +32.6 (c, 0.87 in MeOH).

Butyl ester: [119839-28-0].
$C_{13}H_{18}O_3$ M 222.2 $[\alpha]_D^{20}$ +36 (c, 1 in $CHCl_3$).

Benzyl ester: [119838-72-1].
Liq. $[\alpha]_D^{25}$ +35.4 (c, 1 in $CHCl_3$). n_D^{25} 1.5691.

Nitrile: [101219-69-6].
C_9H_9NO M 147.1 Liq. $[\alpha]_D^{21}$ +41.7 (c, 1.05 in MeOH).

(*S*)-form [125577-89-1]

Et ester: [134615-20-6].
Liq.

(±)-form

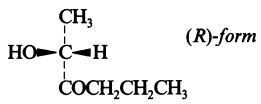
Et ester: [134615-36-4].
Liq.

[107751-31-5]

Eur. Pat., 289 307, (1988); *CA*, **111**, 7063s (*derivs*)
Kusumoto, T. *et al*, *Chem. Lett.*, 1990, 523 (*Me ester, R-form*)
Japan. Pat., 0 262 848, (1990); *CA*, **113**, 201514w.
Japan. Pat., 0 272 140, (1990); *CA*, **113**, 58706c (*esters, use*)
Japan. Pat., 02 268 697, (1990); *CA*, **115**, 47792t (*Et ester, S-, ±-forms*)
Mathre, D.P. *et al*, *J.O.C.*, 1993, **58**, 2880 (*nitrile, Et ester, synth, pmr*)

2-Hydroxy-3-hexanone H-1-00095

[54073-43-7]



(*R*)-form

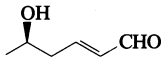
$C_6H_{12}O_2$ M 116.1

(*R*)-form [125850-18-2]
$[\alpha]_D^{22}$ −55.5 (c, 0.7 in $CHCl_3$) (98% ee).

(±)-form [152322-24-2]
Minor component of the male phermone of Hylotrupes bajulus. Oil. Bp_{11} 60-61°. n_D^{20} 1.4245.

Nazarov, I.N. *et al*, *Zh. Obshch. Khim.*, 1957, **27**, 2676; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1957, **27**, 2629 (*synth*)
Russell, G.A. *et al*, *J.A.C.S.*, 1974, **96**, 5830 (*synth*)
Ncobe, S. *et al*, *Tet. Lett.*, 1978, 2345 (*synth*)
Enders, D. *et al*, *Helv. Chim. Acta*, 1989, **72**, 980 (*R-form*)
Francke, W. *et al*, *Annalen*, 1994, 1211 (*synth, pmr, cmr, ms*)

5-Hydroxy-2-hexenal H-1-00096



$C_6H_{10}O_2$ M 114.1

(*R,E*)-form [69830-85-9]
Oil.

Keck, G.E. *et al*, *J.O.C.*, 1994, **59**, 3112 (*synth, pmr, cmr, ir*)

6-Hydroxy-2-hexenoic acid H-1-00097

$HOCH_2CH_2CH_2CH{=}CHCOOH$

$C_6H_{10}O_3$ M 130.1

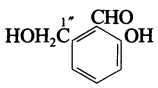
(*E*)-form [38875-88-6]
Cryst. (hexane). Mp 62-63°.

Me ester: [119729-72-5].
$C_7H_{12}O_3$ M 144.1 Oil. $Bp_{0.2}$ 74-76°.

Schore, N.E. *et al*, *J.O.C.*, 1981, **46**, 5357 (*synth, pmr*)
Denmark, S.E. *et al*, *J.O.C.*, 1993, **58**, 1853 (*Me ester, synth*)
Ragoussis, V. *et al*, *Synthesis*, 1993, 84 (*synth*)

2-Hydroxy-6-(hydroxymethyl) benzaldehyde H-1-00098

2-Formyl-3-hydroxybenzyl alcohol



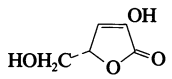
$C_8H_8O_3$ M 152.1
Parent compd. not known (1995).

1″-O-Formyl: [152246-90-7]. *2-Formyl-3-hydroxybenzyl formate*
$C_9H_8O_4$ M 180.1 Isol. from the dust mite, *Dermatophagoides pteronyssinus*. Needles. Mp 59°.

Sato, M. *et al*, *Biosci., Biotechnol., Biochem.*, 1993, **57**, 1299 (*isol, deriv*)

3-Hydroxy-5-hydroxymethyl-2(5*H*)-furanone, 9CI H-1-00099

[152711-16-5]



$C_5H_6O_4$ M 130.1

(*S*)-form
Unstable oil.

O^3-*Me:* [152711-13-2]. *5-Hydroxymethyl-3-methoxy-2(5H)-furanone*
$C_6H_8O_4$ M 144.1 Cryst. (EtOAc/pentane). Mp 84-85°.

O^3-*Benzyl:* [39823-98-8]. *3-Benzyloxy-5-hydroxymethyl-2(5H)-furanone*
$C_{12}H_{12}O_4$ M 220.2 Mp 100-101°. $[\alpha]_D$ +11.4 (c, 1.0 in MeOH).

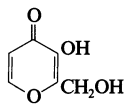
Dibenzyl ether: [55094-61-6].
$C_{19}H_{18}O_4$ M 310.3 Mp 91.5-92.5°. $[\alpha]_D^{20}$ −1.7 (c, 2 in $CHCl_3$).

Linden, A., *Acta Cryst. C*, 1992, **48**, 1514 (*cryst struct, dibenzyl ether*)
Bigorra, J., *Tetrahedron*, 1993, **49**, 6717 (*synth, ir, ms, pmr, cmr*)

3-Hydroxy-2-(hydroxymethyl)-4*H*-pyran-4-one, 9CI H-1-00100

α-Hydroxymaltol

[1968-51-0]



$C_6H_6O_4$ M 142.1
Metab. of *Talaromyces flavus*. Mp 148-150° (146-148°).

1′-Benzoyl: [25552-07-2].
$C_{13}H_{10}O_5$ M 246.2 Mp 136-139°.

1′-O-(4-Hydroxybenzoyl), 3-O-β-D-glucopyranoside: [149573-61-5]. ***Tunicoside***
$C_{19}H_{20}O_{11}$ M 424.3 Constit. of *Tunica prolifera*. Prisms and needles (EtOH). Mp 234°.

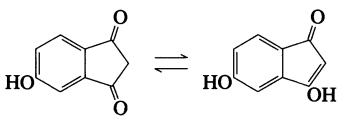
1′-O-(4-Hydroxy-3-methoxybenzoyl), 3-O-β-D-glucopyranoside: ***Methoxytunicoside***
$C_{20}H_{22}O_{12}$ M 454.3 Constit. of *T. prolifera*. Prisms and needles (EtOH). Mp 125°.

3-Me ether: [106203-46-7]. *2-(Hydroxymethyl)-3-methoxy-4H-pyran-4-one, 9CI*
$C_7H_8O_4$ M 156.1 Cryst. (Me_2CO/cyclohexane). Mp 113-115°.

Kingsbury, C.A. *et al*, *J.O.C.*, 1976, **41**, 2777 (*cmr*)
Looker, J.H. *et al*, *J. Het. Chem.*, 1986, **23**, 225 (*synth*)
Ayer, W.A. *et al*, *Can. J. Chem.*, 1990, **68**, 2095 (*isol, pmr*)
Plouvier, V. *et al*, *Phytochemistry*, 1993, **32**, 1618 (*isol, derivs*)

5-Hydroxy-1,3-indanedione H-1-00101

3,5-Dihydroxy-1H-inden-1-one



$C_9H_6O_3$ M 162.1

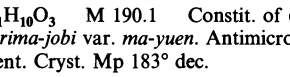
Enol-form

Di-Me ether: [149665-18-9]. *3,5-Dimethoxy-1H-inden-1-one.* ***Coixinden A***
$C_{11}H_{10}O_3$ M 190.1 Constit. of *Coix lacrima-jobi* var. *ma-yuen*. Antimicrobial agent. Cryst. Mp 183° dec.

Ishiguro, Y. *et al*, *Biosci., Biotechnol., Biochem.*, 1993, **57**, 866 (*isol*)

5-Hydroxy-4-isoxazolecarboxylic acid H-1-00102

2,5-Dihydro-5-oxo-4-isoxazolecarboxylic acid, 9CI



$C_4H_3NO_4$ M 129.0

Et ester: [54535-14-7].
$C_6H_7NO_4$ M 157.1 Mp 160.5°, Mp 183.5° (double Mp).

Claisen, L., *Annalen*, 1897, **297**, 1.

2-(Hydroxymethoxy)ethanol, 9CI H-1-00103

[13149-79-6]

$HOCH_2OCH_2CH_2OH$

$C_3H_8O_3$ M 92.0
Used in bactericidal and fungicidal compositions; preservative for lubricating oils. Liq.

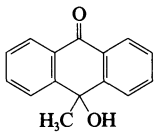
1-Me ether: 2-(*Methoxymethoxy*)*ethanol*
$C_4H_{10}O_3$ M 106.1 Liq. d^{16} 1.04. Bp 150-153°.

1-Ph ether: [148355-61-7]. 2-(*Phenoxymethoxy*)*ethanol, 9CI*
$C_9H_{12}O_3$ M 168.1 Oil. $Bp_{0.2}$ 81-83°.

U.S. Pat., 2 321 608, (1943); *CA*, **37**, 6674[1].
Diehl, K.H. *et al*, *CA*, 1985, **102**, 27791v (*use*)
Romanian Pat., 88 534, (1986); *CA*, **106**, 63013j (*use*)
Aitken, D.J. *et al*, *J.C.S. Perkin 1*, 1993, 597 (*Ph ether*)

10-Hydroxy-10-methyl-9(10*H*)-anthracenone, 9CI H-1-00104

[17104-31-3]



$C_{15}H_{12}O_2$ M 224.2
Mp 146-148°, Mp 153-155° (double Mp).

Ac:
$C_{17}H_{14}O_3$ M 266.2 Needles (EtOH). Mp 104-105°.

Me ether: [53190-24-2]. *10-Methoxy-10-methyl-9(10*H*)-anthracenone*
$C_{16}H_{14}O_2$ M 238.2 Needles (MeOH). Mp 115-116°.

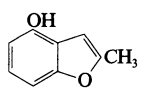
Et ether: [98612-79-4]. *10-Ethoxy-10-methyl-9(10*H*)-anthracenone*
$C_{17}H_{16}O_2$ M 252.3 Oil.

Southern, P.F. *et al*, *J.C.S.*, 1960, 4340 (*synth, ir*)
Bhattacharya, A.K. *et al*, *J.O.C.*, 1983, **48**, 2412 (*synth, ir, pmr*)
Hulinská, H. *et al*, *Coll. Czech. Chem. Comm.*, 1989, **54**, 1388 (*synth, ms, uv, pmr*)
Lin, T. *et al*, *Acta Cryst. C*, 1992, **48**, 1870 (*synth, cryst struct, acetate*)

4-Hydroxy-2-methylbenzofuran H-1-00105

2-Methyl-4-benzofuranol, 9CI

[3610-14-8]



$C_9H_8O_2$ M 148.1
Cryst. (petrol). Mp 54°. Bp_{15} 145-146°.

Ac: [121724-99-0]. *4-Acetoxy-2-methylbenzofuran*
$C_{11}H_{10}O_3$ M 190.1 Prisms (hexane). Mp 50-51°.

Me ether: [3781-89-3]. *4-Methoxy-2-methylbenzofuran*
$C_{10}H_{10}O_2$ M 162.1 Bp_{12} 120°.

Demerseman, P. *et al*, *Bull. Soc. Chim. Fr.*, 1965, 1473 (*Me ether*)
Iwasaki, M. *et al*, *J.O.C.*, 1991, **56**, 1922 (*synth, pmr, Ac*)

4-Hydroxy-3-methylbenzofuran H-1-00106

3-Methyl-4-benzofuranol, 9CI

[3610-15-9]

$C_9H_8O_2$ M 148.1
Needles (C_6H_6/petrol). Mp 110-112°.

Me ether: [3781-88-2]. *4-Methoxy-3-methylbenzofuran*
$C_{10}H_{10}O_2$ M 162.1 Bp_{12} 117°.

Whalley, W.B., *J.C.S.*, 1951, 3229 (*synth*)
Demerseman, P. *et al*, *Bull. Soc. Chim. Fr.*, 1965, 1473 (*synth, Me ether*)
Wasson, B.K. *et al*, *J.O.C.*, 1977, **42**, 4265 (*synth, ir, pmr*)

4-Hydroxy-6-methylbenzofuran H-1-00107

6-Methyl-4-benzofuranol

$C_9H_8O_2$ M 148.1

Ac: [121724-97-8].
$C_{11}H_{10}O_3$ M 190.1 Oil.

Iwasaki, M. *et al*, *J.O.C.*, 1991, **56**, 1922 (*synth, pmr*)

4-Hydroxy-7-methylbenzofuran H-1-00108

7-Methyl-4-benzofuranol, 9CI

$C_9H_8O_2$ M 148.1

Ac: [121724-98-9].
$C_{11}H_{10}O_3$ M 190.1 Prisms (hexane). Mp 49-50°.

Iwasaki, M. *et al*, *J.O.C.*, 1991, **56**, 1922 (*synth, pmr, ir*)

5-Hydroxy-2-methylbenzofuran H-1-00109

2-Methyl-5-benzofuranol, 9CI

[6769-56-8]

$C_9H_8O_2$ M 148.1
Mp 35-36°. Bp_6 134°.

Me ether: [13391-27-0]. *5-Methoxy-2-methylbenzofuran*
$C_{10}H_{10}O_2$ M 162.1 Bp_{10} 117-118°.

Grinev, A.N. *et al*, *Zh. Obshch. Khim.*, 1957, **27**, 1087; *CA*, **52**, 3761f (*synth*)

5-Hydroxy-3-methylbenzofuran H-1-00110

3-Methyl-5-benzofuranol, 9CI

[7182-21-0]

$C_9H_8O_2$ M 148.1
Cryst. Mp 93-94°.

Whalley, W.B., *J.C.S.*, 1953, 3479 (*synth*)
Domschke, G., *J. Prakt. Chem.*, 1966, **32**, 144 (*synth*)
Lee, J. *et al*, *J.O.C.*, 1990, **55**, 4995 (*synth, ir, pmr, cmr, bibl*)

6-Hydroxy-2-methylbenzofuran H-1-00111

2-Methyl-6-benzofuranol, 9CI

[54584-24-6]

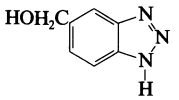
$C_9H_8O_2$ M 148.1
Mp 74.5°.

Baxter, G.J. *et al*, *Aust. J. Chem.*, 1974, **27**, 2605 (*synth, pmr, ir, uv*)

5(6)-(Hydroxymethyl)benzotriazole H-1-00112

1H-Benzotriazole-5-methanol, 9CI

[106429-67-8]



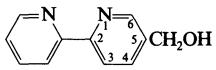
$C_7H_7N_3O$ M 149.1
Mp 149-150°.

Katritzky, A.R. *et al*, *Synth. Commun.*, 1993, **23**, 2019 (*synth, pmr, cmr*)

5-(Hydroxymethyl)-2,2′-bipyridine H-1-00113

[*2,2′-Bipyridine*]-*5-methanol, 9CI*

[146581-87-5]



$C_{11}H_{10}N_2O$ M 186.2
Thick orange oil.

Imperiali, B. *et al*, *J.O.C.*, 1993, **58**, 1613 (*synth*)

6-(Hydroxymethyl)-2,2′-bipyridine H-1-00114

[*2,2′-Bipyridine*]-*6-methanol, 9CI*

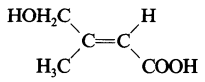
[149775-41-7]

$C_{11}H_{10}N_2O$ M 186.2
Oil.

Uenishi, J. *et al*, *J.O.C.*, 1993, **58**, 4382 (*synth, pmr, ir, cmr, ms*)

4-Hydroxy-3-methyl-2-butenoic acid, 9CI H-1-00115

4-Hydroxy-3-methylcrotonic acid



(*E*)-*form*

$C_5H_8O_3$ M 116.1

(*E*)-*form* [44647-19-0]
Needles (C_6H_6). Mp 112-113° (108-110°).

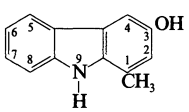
Me ester: [13866-57-4].
$C_6H_{10}O_3$ M 130.1 Bp_1 30-50°.

Ac: [21622-85-5].
$C_7H_{10}O_4$ M 158.1 Bp_{12} 154-155°.

Nechvatal, A. *et al*, *J.C.S.(C)*, 1968, 185 (*synth*)
Bourguignon, J.-J. *et al*, *J. Med. Chem.*, 1988, **31**, 893 (*synth, pmr*)
Schmidt, R.R. *et al*, *Synthesis*, 1994, 255 (*synth, Ac, pmr*)

3-Hydroxy-1-methyl-9*H*-carbazole H-1-00116

1-Methyl-9H-carbazol-3-ol



$C_{13}H_{11}NO$ M 197.2

Cryst. Mp >158° dec.

Knölker, H.-J. *et al*, *Synthesis*, 1995, 397 (*synth, uv, ir, pmr, cmr, ms*)

3-Hydroxy-2-methyl-9*H*-carbazole H-1-00117

*2-Methyl-9*H*-carbazol-3-ol*

$C_{13}H_{11}NO$ M 197.2
Needles (C_6H_6). Mp 276°.

Me ether: [6933-09-1]. *3-Methoxy-2-methyl-9*H*-carbazole*
$C_{14}H_{13}NO$ M 211.2 Needles (EtOH). Mp 179-181.5°.

Cummins, J.A. *et al*, *J.C.S.*, 1954, 1414 (*synth, Me ether*)
Knölker, H.-J. *et al*, *Synthesis*, 1995, 397 (*synth, uv, ir, pmr, cmr, ms*)

3-Hydroxy-5-methyl-9*H*-carbazole H-1-00118

*5-Methyl-9*H*-carbazol-3-ol, 9CI*

[77120-62-8]

$C_{13}H_{11}NO$ M 197.2
Flakes (xylene). Mp 200°.

Bisagni, E. *et al*, *Tetrahedron*, 1980, **36**, 1327 (*synth, ir, pmr*)

3-Hydroxy-7-methyl-9*H*-carbazole H-1-00119

*7-Methyl-9*H*-carbazol-3-ol, 9CI*

[61601-53-4]

$C_{13}H_{11}NO$ M 197.2
Cryst. (EtOH aq. or PhCl). Mp 250-253° dec.

Stetter, H. *et al*, *Annalen*, 1958, **617**, 54 (*synth*)
Chowdhury, B.K. *et al*, *CA*, 1977, **86**, 121578d (*synth*)

3-Hydroxy-8-methyl-9*H*-carbazole H-1-00120

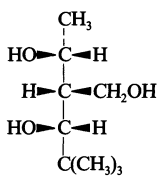
*8-Methyl-9*H*-carbazol-3-ol, 9CI*

[61601-52-3]

$C_{13}H_{11}NO$ M 197.2
Mp 175°.

Chowdhury, B.K. *et al*, *CA*, 1977, **86**, 121578d (*synth*)

3-Hydroxymethyl-5,5-dimethyl-2,4-hexanediol H-1-00121



$C_9H_{20}O_3$ M 176.2

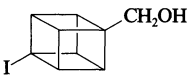
(2R,3S,4R)-form [147673-38-9]
Triol contg. 3 OH groups in different chiral environments. Prototype of a series of starting materials for synth. of dendrimers contg. a chiral core. Solid.

Seebach, D. *et al*, *Helv. Chim. Acta*, 1994, **77**, 1673.

1-Hydroxymethyl-4-iodocubane H-1-00122

4-Iodopentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octanemethanol, 9CI

[163332-87-4]



C_9H_9IO M 260.0
Cryst. (hexane). Mp 108-110°.

Eaton, P.E. *et al*, *J.A.C.S.*, 1994, **116**, 7588 (*synth, pmr, cmr*)

(Hydroxymethyl)methylcarbamodithioic acid, 9CI H-1-00123

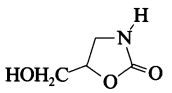
$HOCH_2NMeC(S)SH$

$C_3H_7NOS_2$ M 137.2

K salt: [51026-28-9]. *Bunema. Busan 40*
Bactericide and wood preservative.

Netherlands Pat., 7 602 496, (1977); *CA*, **89**, 100994h (*synth, use*)

5-Hydroxymethyl-2-oxazolidinone H-1-00124



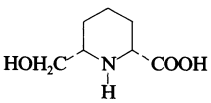
$C_4H_7NO_3$ M 117.1

(±)-form
Solid. Mp 71-72°.

O-(4-Methylbenzenesulfonyl): Solid. Mp 98-99°.

Seneci, P. *et al*, *J.C.S. Perkin 1*, 1994, 2345.

6-(Hydroxymethyl)-2-piperidinecarboxylic acid, 9CI H-1-00125



$C_7H_{13}NO_3$ M 159.1

(2RS,6SR)-form [161431-60-3]
(±)-cis-*form*
Hygroscopic solid. Mp 231-233° dec.

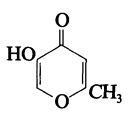
Et ester:
$C_9H_{17}NO_3$ M 187.2 Cryst. (EtOH). Mp 196-198°.

Bolós, J. *et al*, *J. Het. Chem.*, 1994, **31**, 1493 (*synth, ir, pmr*)

5-Hydroxy-2-methyl-4*H*-pyran-4-one, 9CI H-1-00126

α-Deoxykojic acid. Allomaltol

[644-46-2]



$C_6H_6O_3$ M 126.1
Cryst. (EtOAc). Mp 153-154°.

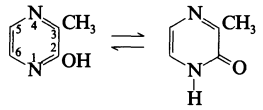
Ac: [54917-86-1].
$C_8H_8O_4$ M 168.1 Cryst. (Et_2O/petrol). Mp 103°.

Brockhaus, M. *et al*, *Annalen*, 1974, 1675 (*synth, uv, pmr*)
Arnarp, J., *Acta Chem. Scand.*, 1990, **44**, 916 (*synth, pmr, ms*)

2-Hydroxy-3-methylpyrazine H-1-00127

*3-Methyl-2(1*H*)-pyrazinone, 9CI. 3-Methylpyrazinol, 8CI*

[19838-07-4]



$C_5H_6N_2O$ M 110.1
Cryst. (EtOAc). Mp 151-152°.

Karmus, G. *et al*, *J.A.C.S.*, 1952, **74**, 1580 (*synth*)
Macdonald, J.C. *et al*, *Tetrahedron*, 1976, **32**, 655 (*pmr, cmr*)

2-Hydroxy-5-methylpyrazine H-1-00128

*5-Methyl-2(1*H*)-pyrazinone, 9CI. 5-Methylpyrazinol, 8CI*

[20721-17-9]

$C_5H_6N_2O$ M 110.1
Cryst. Mp 68-69°, Mp 126-128°.

Karmus, G. *et al*, *J.A.C.S.*, 1952, **74**, 1580 (*synth*)
Koelsch, C.F. *et al*, *J.O.C.*, 1958, **23**, 1603 (*synth*)
Macdonald, J.C. *et al*, *Tetrahedron*, 1976, **32**, 655 (*pmr, cmr*)

2-Hydroxy-6-methylpyrazine H-1-00129

*6-Methyl-2(1*H*)-pyrazinone, 9CI. 6-Methylpyrazinol, 8CI*

[20721-18-0]

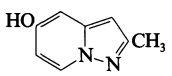
$C_5H_6N_2O$ M 110.1
Cryst. (H_2O). Mp 250-251°.

Karmus, G. *et al*, *J.A.C.S.*, 1952, **74**, 1580 (*synth*)
Macdonald, J.C. *et al*, *Tetrahedron*, 1976, **32**, 655 (*pmr, cmr*)

5-Hydroxy-2-methylpyrazolo[1,5-*a*]pyridine H-1-00130

2-Methylpyrazolo[1,5-a]pyridin-5-ol

[156969-44-7]



$C_8H_8N_2O$ M 148.1
Yellow solid by subl. Mp 186-187° dec.

Ac: [156969-45-8].
$C_{10}H_{10}N_2O_2$ M 190.2 Fine needles by subl. Mp 68-69°.

Benzoyl: [156969-46-9].
$C_{15}H_{12}N_2O_2$ M 252.2 Cryst. (hexane).

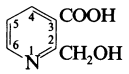
Me ether: [156969-47-0]. *5-Methoxy-2-methylpyrazolo[1,5-a]pyridine*
$C_9H_{10}N_2O$ M 162.1 Oil.

Brown, R.F.C. *et al*, *Aust. J. Chem.*, 1994, **47**, 1009 (*synth, pmr, cmr, cryst struct, props*)

2-(Hydroxymethyl)-3-pyridinecarboxylic acid, 9CI H-1-00131

2-(Hydroxymethyl)nicotinic acid, 8CI

[81113-14-6]



$C_7H_7NO_3$ M 153.1
Cryst. (EtOH). Mp 153-154° dec.

Ac, Me ester:
$C_{10}H_{11}NO_4$ M 209.2 Oil.

Ac, Et ester: [31181-70-1].
$C_{11}H_{13}NO_4$ M 223.2 $Bp_{1.0}$ 122-127°.

Sato, Y. *et al, Chem. Pharm. Bull.*, 1960, **8**, 427 (*synth, ir, uv, pmr, ms*)
Blanz, E.J. *et al, J. Med. Chem.*, 1970, **13**, 1124 (*Ac-Et ester*)
Matsuura, I., *Heterocycles*, 1975, **3**, 381 (*Ac-Me ester*)
Ashcroft, W.R. *et al, J.C.S. Perkin 1*, 1981, 3012 (*synth, uv, ir, pmr, ms*)

2-(Hydroxymethyl)-4-pyridinecarboxylic acid, 9CI H-1-00132

2-(Hydroxymethyl)isonicotinic acid, 8CI

$C_7H_7NO_3$ M 153.1

Me ester: [58481-17-7].
$C_8H_9NO_3$ M 167.1 Mp 68-69°.

Amide: [84589-39-9].
$C_7H_8N_2O_2$ M 152.1 Mp 183-184.5°.

Sugiyama, T. *et al, Bull. Chem. Soc. Jpn.*, 1982, **55**, 3055; 1984, **57**, 1882.

3-(Hydroxymethyl)-2-pyridinecarboxylic acid, 9CI H-1-00133

3-(Hydroxymethyl)picolinic acid

$C_7H_7NO_3$ M 153.1

Ac, Et ester: [56526-05-7].
$C_{11}H_{13}NO_4$ M 223.2 Oil.

Lactone: see *Furo[3,4-b]pyridin-7(5H)-one, F-0-01473*

Matsuura, I., *Heterocycles*, 1975, **3**, 381 (*Ac-Et ester*)

3-(Hydroxymethyl)-4-pyridinecarboxylic acid, 9CI H-1-00134

3-(Hydroxymethyl)isonicotinic acid

[81113-13-5]

$C_7H_7NO_3$ M 153.1
Gummy solid.

Lactone: see *Furo[3,4-c]pyridin-1(3H)-one, F-0-01476*

Ashcroft, W.R. *et al, J.C.S. Perkin 1*, 1981, 3012 (*synth, uv, ir, pmr, ms*)

4-(Hydroxymethyl)-2-pyridinecarboxylic acid, 9CI H-1-00135

4-(Hydroxymethyl)picolinic acid

$C_7H_7NO_3$ M 153.1

Et ester: [59663-96-6].
$C_9H_{11}NO_3$ M 181.1 Cryst. (Et_2O/hexane). Mp 78-79°.

Hutchison, A.J. *et al, J. Med. Chem.*, 1989, **32**, 2171.
El Hadri, A. *et al, J. Het. Chem.*, 1993, **30**, 631.

4-(Hydroxymethyl)-3-pyridinecarboxylic acid, 9CI H-1-00136

4-(Hydroxymethyl)nicotinic acid, 8CI

[72726-63-7]

$C_7H_7NO_3$ M 153.1
Gummy solid. Unstable, lactonises rapidly.

Nitrile: [157650-27-6].
$C_7H_6N_2O$ M 134.1 Cryst. (EtOH/Et_2O). Mp 143°.

Ac, Me ester: [55768-93-9].
$C_{10}H_{11}NO_4$ M 209.2 Oil. $Bp_{0.5}$ 140-150°.

Lactone: see *Furo[3,4-c]pyridin-3(1H)-one, F-0-01477*

Battaro, J.C. *et al, J.O.C.*, 1980, **45**, 1176 (*synth*)
Ashcroft, W.R. *et al, J.C.S. Perkin 1*, 1981, 3012 (*synth, uv, ir, pmr, ms*)

5-(Hydroxymethyl)-2-pyridinecarboxylic acid, 9CI H-1-00137

5-(Hydroxymethyl)picolinic acid

[39977-41-8]

$C_7H_7NO_3$ M 153.1
Mp 216°.

Et ester: [50501-35-4].
$C_9H_{11}NO_3$ M 181.1 Mp 67°.

Dawson, M.I., *J. Med. Chem.*, 1983, **26**, 1282 (*synth, ir, pmr*)

5-(Hydroxymethyl)-3-pyridinecarboxylic acid, 9CI H-1-00138

5-(Hydroxymethyl)nicotinic acid

$C_7H_7NO_3$ M 153.1

Et ester: [59936-06-0].
$C_9H_{11}NO_3$ M 181.1 Oil. $Bp_{0.01}$ 136°.

Amide: [59936-07-1].
$C_7H_8N_2O_2$ M 152.1 Cryst. (EtOH). Mp 158°.

Trommer, W.E. *et al, Annalen*, 1976, 848.

6-(Hydroxymethyl)-2-pyridinecarboxylic acid, 9CI H-1-00139

6-(Hydroxymethyl)picolinic acid, 8CI

[1197-10-0]

$C_7H_7NO_3$ M 153.1
Cryst. (Me_2CO). Mp 152° (137°).

Me ester: [39977-44-1].
$C_8H_9NO_3$ M 167.1 Mp 88°.

Et ester: [41337-81-9].
$C_9H_{11}NO_3$ M 181.1 Cryst. (EtOH/Et_2O). Mp 95-96°, Mp 131-133°.

Ac: [80540-79-0].
$C_9H_9NO_4$ M 195.1 Cryst. (C_6H_6). Mp 113-115° dec.

Ac, Et ester:
$C_{11}H_{13}NO_4$ M 223.2 Oil.

N-*Oxide:* [24191-19-3].
$C_7H_7NO_4$ M 169.1 Mp 195°.

Mathes, W. *et al, Chem. Ber.*, 1953, **86**, 1953 (*synth*)
Fife, T.H. *et al, J.A.C.S.*, 1982, **104**, 2251 (*synth*)
Bolós, J. *et al, J. Het. Chem.*, 1994, **31**, 1493 (*synth, pmr*)
Vergopoulos, V. *et al, Z. Naturforsch., B*, 1994, **49**, 1127 (*synth, ir, pmr, cmr*)

6-(Hydroxymethyl)-3-pyridinecarboxylic acid H-1-00140

6-(Hydroxymethyl)nicotinic acid

$C_7H_7NO_3$ M 153.1

Et ester: [35005-81-3].
$C_9H_{11}NO_3$ M 181.1 Mp 67°. $Bp_{0.5}$ 86°.

Ac, Me ester: [63362-34-5].
$C_{10}H_{11}NO_4$ M 209.2 Mp 88°. Bp_3 117-120°.

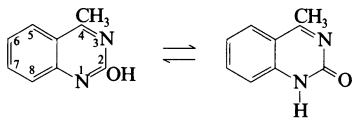
Ac, Et ester:
$C_{11}H_{13}NO_4$ M 223.2 Needles. Mp 25°. $Bp_{0.5}$ 138°.

Morris, I.G. *et al, J.C.S.*, 1963, 1841.

2-Hydroxy-4-methylquinazoline H-1-00141

4-Methyl-2(1H)-quinazolinone, 9CI. 4-Methyl-2-quinazolinol

[34790-24-4]



$C_9H_8N_2O$ M 160.1
CAS. no. refers to the oxo-form. Cryst. (DMF/EtOH). Mp 230-232°.

Armarego, W.L.F. *et al, J.C.S.(C)*, 1966, 234 (*synth*)
Yamamoto, M. *et al, Chem. Pharm. Bull.*, 1978, **26**, 1633 (*synth*)

4-Hydroxy-5-methylquinazoline H-1-00142

5-Methyl-4(1H)-quinazolinone, 9CI. 5-Methyl-4-quinazolinol

[75844-41-6]

$C_9H_8N_2O$ M 160.1
CAS no. refers to the oxo-tautomer. Needles (H_2O). Mp 225-227° (210-212°).

Baker, B.R. *et al, J.O.C.*, 1952, **17**, 141 (*synth*)
Gupton, J.T. *et al, Synth. Commun.*, 1984, **14**, 1013 (*synth, ir, pmr*)

4-Hydroxy-6-methylquinazoline H-1-00143

6-Methyl-4(1H)-quinazolinone, 9CI. 6-Methyl-4-quinazolinol

[19181-53-4]

$C_9H_8N_2O$ M 160.1
CAS no. refers to the oxo-tautomer. Cryst. (EtOH). Mp 258° (242°).

Baker, B.R. *et al, J.O.C.*, 1952, **17**, 141 (*synth*)
Gupton, J.T. *et al, Synth. Commun.*, 1984, **14**, 1013 (*synth, ir, pmr*)
Stevenson, T.M. *et al, J.O.C.*, 1986, **51**, 616 (*synth*)

4-Hydroxy-7-methylquinazoline H-1-00144

7-Methyl-4(1H)-quinazolinone, 9CI. 7-Methyl-4-quinazolinol

[75844-40-5]

$C_9H_8N_2O$ M 160.1
CAS no. refers to the oxo-tautomer. Needles (EtOH). Mp 239-240°.

Baker, B.R. *et al, J.O.C.*, 1952, **17**, 141 (*synth*)

4-Hydroxy-8-methylquinazoline H-1-00145

8-Methyl-4(1H)-quinazolinone, 9CI. 8-Methyl-4-quinazolinol

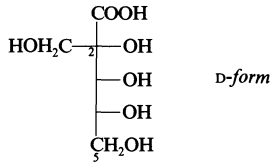
[19181-54-5]

$C_9H_8N_2O$ M 160.1
Needles (EtOH). Mp 264-267° (251°).

Baker, B.R. *et al, J.O.C.*, 1952, **17**, 141 (*synth*)
Gupton, J.T. *et al, Synth. Commun.*, 1984, **14**, 1013 (*synth, ir, pmr*)

2-*C*-(Hydroxymethyl)ribonic acid, 9CI H-1-00146

2-Carboxyarabinitol. Hamamelonic acid



D-*form*

$C_6H_{12}O_7$ M 196.1

D-form [469-09-0]
Constit. of numerous plant spp. Needles (MeOH aq.) (asNH_4 salt). Mp 152° (NH_4 salt). $[\alpha]_D$ −3.9 (c, 10 in H_2O).

5-O-Phosphate: [112160-91-5].
$C_6H_{13}O_{10}P$ M 276.1 Isol. from the leaves of *Phaseolus vulgaris*. Inhibitor of ribulose 1,5-bisphosphate carboxylase.

L-form
Needles (MeOH aq.) (as NH_4 salt). Mp 151-152° (NH_4 salt). $[\alpha]_D$ +4.8 (c, 1.2 in 1*M* NH_4OH).

γ-Lactone:
$C_6H_{10}O_6$ M 178.1 Plates (MeCN/$CHCl_3$). Mp 88-89°. $[\alpha]_D$ −74 (c, 2.1 in H_2O).

γ-Lactone, tetra-Ac:
$C_{14}H_{18}O_{10}$ M 346.2 Cryst. (EtOH). Mp 103-104°. $[\alpha]_D$ −102 (c, 1.6 in $CHCl_3$).

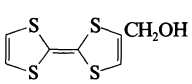
[98587-21-4, 122907-93-1]

Ferrier, R.J., *J.C.S.*, 1962, 3544 (*synth*)
Burton, J.S. *et al, J.C.S.*, 1965, 3433 (*synth*)
Thanbichler, A. *et al, Z. Naturforsch., B*, 1971, **26**, 912 (*synth*)
Gutteridge, S. *et al, Biochem. J.*, 1989, **260**, 711 (*synth*)
Beck, E. *et al, Plant Physiol.*, 1989, **90**, 13 (*pmr, cmr*)
Moore, B.D. *et al, Phytochemistry*, 1993, **34**, 703 (*occur*)

2-(Hydroxymethyl) tetrathiafulvalene H-1-00147

2-(1,3-Dithiol-2-ylidene)-1,3-dithiole-4-methanol, 9CI

[68128-93-8]



$C_7H_6OS_4$ M 234.3
Used in the study of electrically conducting charge - transfer salts. Yellow cryst. (isooctane/toluene). Mp 70-71°. Dec. on standing in air.

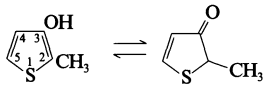
Ac:
$C_9H_8O_2S_4$ M 276.4 Orange solid. Mp 94-95°.

Green, D.C., *J.O.C.*, 1979, **44**, 1476 (*synth, ir, pmr, uv*)
Garín, J. *et al, Synthesis*, 1994, 489 (*synth, Ac, cmr, pmr*)

3-Hydroxy-2-methylthiophene H-1-00148

2-Methylthiophen-3(2H)-one, 9CI. 2-Methylthiophene-3-ol, 9CI

[3760-22-3]



C_5H_6OS M 114.1
Mixt. of tautomers in soln. Liq. Bp_{12} 92-98°, $Bp_{0.2}$ 76-78°. n_D^{20} 1.5460.

Ac:
$C_7H_8O_2S$ M 156.2 Liq. Bp_{10} 86°. n_D^{20} 1.5123.

[3760-25-6]

Hornfeldt, A.B., *Acta Chem. Scand.*, 1965, **19**, 1249 (*synth, tautom, pmr*)
Hunter, G.A. *et al, J.C.S. Perkin 1*, 1995, 1209 (*synth, pmr, cmr*)

4-Hydroxy-2-methylthiophene H-1-00149

5-Methylthiophen-3(2H)-one, 9CI. 5-Methylthiophene-3-ol, 9CI

[128889-82-7]

C_5H_6OS M 114.1
$Bp_{0.2}$ 57-59°.

[121781-88-2]

Hunter, G.A. *et al, J.C.S. Perkin 1*, 1995, 1209 (*synth, pmr, cmr, ms*)

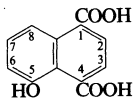
4-Hydroxy-3-methylthiophene H-1-00150

4-Methylthiophen-3(2H)-one. 4-Methylthiophene-3-ol

C_5H_6OS M 114.1
$Bp_{0.1}$ 56-58°. n_D^{20} 1.5589.

Mühlstädt, M. *et al, Chem. Ber.*, 1968, **101**, 1052 (*synth*)

5-Hydroxy-1,4-naphthalenedicarboxylic acid H-1-00151



$C_{12}H_8O_5$ M 232.1

Dinitrile: 5,8-Dicyano-1-naphthol
$C_{12}H_6N_2O$ M 194.1 Light yellow prisms. Mp 273-277°.

Dinitrile, Ac:
$C_{14}H_8N_2O_2$ M 236.2 Yellow prisms. Mp 147-149°.

Tolbert, L.M. *et al, J.A.C.S.*, 1994, **116**, 10593.

6-Hydroxy-1,4-naphthalenedicarboxylic acid H-1-00152

$C_{12}H_8O_5$ M 232.1

Dinitrile: 5,8-Dicyano-2-naphthol
$C_{12}H_6N_2O$ M 194.1 Light yellow solid. Mp 300-310° dec.

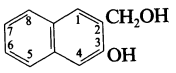
Me ether, dinitrile: 1,4-Dicyano-6-methoxynaphthalene
$C_{13}H_8N_2O$ M 208.2 Prisms. Mp 217-218°.

Tolbert, L.M. *et al, J.A.C.S.*, 1994, **116**, 10593.

3-Hydroxy-2-naphthalenemethanol, 9CI, 8CI H-1-00153

3-Hydroxymethyl-2-naphthol

[30159-70-7]



$C_{11}H_{10}O_2$ M 174.1
Cryst. (EtOH). Mp 188-189°.

Miller, L.E. *et al, J.A.C.S.*, 1954, **76**, 296 (*synth*)
Emmott, P. *et al, J.C.S.*, 1957, 3144 (*synth*)
Przhiyalgovskaya, N.M. *et al, Zh. Obshch. Khim.*, 1961, **31**, 2321 (*synth*)

4-Hydroxy-2-naphthalenemethanol, 9CI, 8CI H-1-00154

3-Hydroxymethyl-1-naphthol

$C_{11}H_{10}O_2$ M 174.1
Mp 98-99°.

Di-Ac:
$C_{15}H_{14}O_4$ M 258.2 Mp 76-78°.

Yares'ko, N.S. *et al, Zh. Obshch. Khim.*, 1964, **34**, 1250; *CA*, **61**, 3041f (*synth*)

8-Hydroxy-1-naphthalenemethanol, 9CI, 8CI H-1-00155

8-Hydroxymethyl-1-naphthol

[18500-91-9]

$C_{11}H_{10}O_2$ M 174.1
Needles (C_6H_6/Me_2CO). Mp 144-146°.

1'-Ac: [35689-24-8].
$C_{13}H_{12}O_3$ M 216.2 Prisms (C_6H_6). Mp 113-114°.

Di-Ac: [35688-95-0].
$C_{15}H_{14}O_4$ M 258.2 Cryst. (C_6H_6/petrol). Mp 81-83°.

8-Me ether: [19190-42-2]. *8-Methoxy-1-naphthalenemethanol, 9CI*
$C_{12}H_{12}O_2$ M 188.2 Cryst. (C_6H_6). Mp 88-90°.

Packer, R.J. *et al, J.C.S.(C)*, 1967, 2194 (*synth*)
Berry, D. *et al, J.C.S. Perkin 1*, 1972, 699 (*synth, derivs, ir, uv*)

1-Hydroxy-7-nitroisoquinoline H-1-00156

7-Nitro-1(2H)-isoquinolinone. 7-Nitroisocarbostyril, 8CI. 7-Nitro-1-isoquinolinol

[20141-83-7]

$C_9H_6N_2O_3$ M 190.1
Cryst. (MeOH or Me_2CO). Mp 265-267° (253-254°).

NH-form
N-*Me:* [54931-51-0]. *2-Methyl-7-nitro-1(2H)-isoquinolinone*
$C_{10}H_8N_2O_3$ M 204.1 Orange needles (EtOH). Mp 214-216°.

Kawazoe, Y. *et al, Chem. Pharm. Bull.*, 1968, **16**, 715 (*synth*)

Henry, R.A. *et al*, *J.O.C.*, 1975, **40**, 1760 (*N-Me*)
Sugimoto, A. *et al*, *Synthesis*, 1995, 431 (*synth, N-Me, ir, pmr, ms*)

3-Hydroxy-2-nitropropanoic acid, 9CI H-1-00157

2-Nitrohydracrylic acid, 8CI

$HOCH_2CH(NO_2)COOH$

$C_3H_5NO_5$ M 135.0

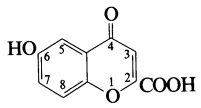
Et ester: [96040-01-6].
$C_5H_9NO_5$ M 163.1 Liq. Bp_2 102-103°, $Bp_{0.06}$ 85°.

Bavievskii, K.K. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1965, **160**, 105; *CA*, **62**, 11702e (*synth*)
Eyer, M. *et al*, *J.A.C.S.*, 1985, **107**, 3601 (*synth, ir, pmr, ms*)
Rozen, S. *et al*, *J.O.C.*, 1994, **59**, 1208 (*synth*)

6-Hydroxy-4-oxo-4*H*-1-benzopyran-2-carboxylic acid H-1-00158

6-Hydroxychromone-2-carboxylic acid

[14718-40-2]



$C_{10}H_6O_5$ M 206.1
Yellow needles (EtOH). Mp 297° (293-294°) dec.

Stoermer, M.J. *et al*, *Aust. J. Chem.*, 1995, **48**, 677 (*synth, pmr, cmr*)

7-Hydroxy-4-oxo-4*H*-1-benzopyran-2-carboxylic acid H-1-00159

7-Hydroxychromone-2-carboxylic acid

[30113-83-8]

$C_{10}H_6O_5$ M 206.1

*Me ether: 7-Methoxy-4-oxo-4*H*-1-benzopyran-2-carboxylic acid*
$C_{11}H_8O_5$ M 220.1 Mp 274-276° dec. (265°).

Stoermer, M.J. *et al*, *Aust. J. Chem.*, 1995, **48**, 677 (*synth, pmr, cmr*)

8-Hydroxy-4-oxo-4*H*-1-benzopyran-2-carboxylic acid H-1-00160

8-Hydroxychromone-2-carboxylic acid

[129472-71-5]

$C_{10}H_6O_5$ M 206.1
Needles + 2 H_2O (EtOH). Mp 254-255° dec.

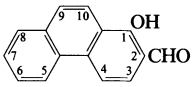
*Me ether: 8-Methoxy-4-oxo-4*H*-1-benzopyran-2-carboxylic acid*
$C_{11}H_8O_5$ M 220.1 Cream needles (EtOH). Mp 260-262° dec. (247-249°).

Stoermer, M.J. *et al*, *Aust. J. Chem.*, 1995, **48**, 677 (*synth, pmr, cmr*)

1-Hydroxy-2-phenanthrenecarboxaldehyde H-1-00161

2-Formyl-1-phenanthrol

[59292-76-1]



$C_{15}H_{10}O_2$ M 222.2
Pale yellow leaflets. Mp 128°.

Cagniant, P. *et al*, *C. R. Hebd. Seances Acad. Sci. Ser. C*, 1976, **282**, 465 (*synth*)

3-Hydroxy-4-phenanthrenecarboxaldehyde H-1-00162

4-Formyl-3-phenanthrol

[10386-43-3]

$C_{15}H_{10}O_2$ M 222.2
Cryst. (Et_2O/petrol). Mp 98°.

Zawadowski, T., *CA*, 1967, **67**, 53915s (*synth*)

3-Hydroxy-9-phenanthrenecarboxaldehyde H-1-00163

9-Formyl-3-phenanthrol

[17850-73-6]

$C_{15}H_{10}O_2$ M 222.2
Cryst. ($CHCl_3$/petrol). Mp 113-114.5°.

Bronovitskaya, V.P. *et al*, *Zh. Org. Khim.*, 1968, **4**, 340.

4-Hydroxy-3-phenanthrenecarboxaldehyde H-1-00164

3-Formyl-4-phenanthrol

[59292-77-2]

$C_{15}H_{10}O_2$ M 222.2
Yellow-brown leaflets. Mp 109°.

Cagniant, P. *et al*, *C. R. Hebd. Seances Acad. Sci. Ser. C*, 1976, **282**, 465 (*synth*)

10-Hydroxy-9-phenanthrenecarboxaldehyde H-1-00165

10-Formyl-9-phenanthrol

[16278-20-9]

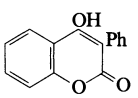
$C_{15}H_{10}O_2$ M 222.2
Yellow cryst. (EtOH or $CHCl_3$/petrol). Mp 135-136°.

Litinas, K.E. *et al*, *J.C.S. Perkin 1*, 1985, 429 (*synth, pmr, ms*)
Alarcón, S.H. *et al*, *Tetrahedron*, 1995, **51**, 4619 (*synth, ir, pmr, cmr, ms*)

4-Hydroxy-3-phenyl-2*H*-1-benzopyran-2-one, 9CI H-1-00166

4-Hydroxy-3-phenylcoumarin

[1786-05-6]



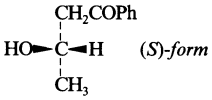
$C_{15}H_{10}O_3$ M 238.2
Needles ($MeOH/C_6H_6$). Mp 238-239°.

Geoghegan, M. *et al*, *Tetrahedron*, 1966, **22**, 3209 (*synth, uv*)
Kirkiacharian, B.S. *et al*, *C. R. Hebd. Seances Acad. Sci. Ser. C*, 1977, **284**, 697 (*cmr*)
Barton, D.H.R. *et al*, *J.C.S. Perkin 1*, 1992, 1365 (*ir, ms, pmr*)
Clerici, A. *et al*, *Synthesis*, 1993, 99 (*synth, ir, ms*)

3-Hydroxy-1-phenyl-1-butanone, 9CI H-1-00167

3-Hydroxybutyrophenone, 8CI. 1-Benzoyl-2-propanol

[13505-39-0]



$C_{10}H_{12}O_2$ M 164.2

(S)-form [105735-20-4]
Oil. $[\alpha]_D^{24}$ +68.4 (c, 3.6 in $CHCl_3$) (98% ee).

(±)-form [105927-50-2]
Oil. Bp_{12} 150-151°.

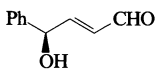
2,4-Dinitrophenylhydrazone: Cryst. (EtOH). Mp 178-179°.

Semicarbazone: Mp 153-154°.

[116660-74-3]

Staudinger, H. *et al*, *Annalen*, 1911, **384**, 124 (*synth*)
Baldwin, J.E. *et al*, *J.C.S.*, 1962, 4743 (*synth, uv*)
Fauve, A. *et al*, *J.O.C.*, 1988, **54**, 5215 (*synth, pmr, bibl*)
Takeshita, M. *et al*, *J.C.S. Perkin 1*, 1993, 2901 (*synth, pmr,*)

4-Hydroxy-4-phenyl-2-butenal, 9CI H-1-00168



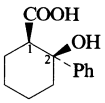
$C_{10}H_{10}O_2$ M 162.1

(2E,4R)-form [147513-34-6]
$[\alpha]_D^{25}$ +222.9 (c, 0.79 in $CHCl_3$) (95% ee).

Yu, L. *et al*, *Chem. Comm.*, 1993, 232 (*synth*)

2-Hydroxy-2-phenylcyclohexanecarboxylic acid, 9CI H-1-00169

Cicloxilic acid, INN. Plecton. Sintiabil



(1R,2S)-form

$C_{13}H_{16}O_3$ M 220.2
Choleretic agent; used to treat liver disorders. Starting material used in synth. of dialkylaminoethyl or aminocycloalkyl esters (spasmolytic agents).

(1R,2S)-form [154098-18-7]
(+)-cis-*form*
Cryst. (EtOH aq.). $[\alpha]_D$ +12.88 (c, 1 in 0.5*M* NaOH) (98% ee).

(1S,2R)-form [154028-93-0]
(−)-cis-*form*
Cryst. Mp 135-137°. $[\alpha]_D$ −12.7 (c, 1 in 0.5*M* NaOH) (98% ee).

(1RS,2SR)-form [57808-63-6]
(±)-cis-*form*
Mp 145-147°.

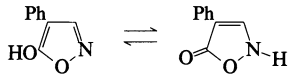
▶ LD_{50} (rat, orl) 1570 mg/kg. LD_{50} (rat, ipr) 1040 mg/kg. GU8582800.

Zimmermann, H. *et al*, *J.A.C.S.*, 1954, **76**, 2285 (*synth*)
Ger. Pat., 2 427 290, (1975) (*Guidotti Internat*); *CA*, **84**, 43643p (*synth*)
Bramanti, G. *et al*, *Arzneim.-Forsch.*, 1978, **28**, 1205 (*props, pharmacol, config, pmr, ir*)
De Angelis, L., *Drugs of Today (Barcelona)*, 1979, **15**, 163 (*rev*)
Subissi, A. *et al*, *Arzneim.-Forsch.*, 1982, **32**, 1310 (*activity*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 1353.
Salvadori, P. *et al*, *Tetrahedron*, 1994, **50**, 205 (*abs config, cd, synth*)

5-Hydroxy-4-phenylisoxazole H-1-00170

4-Phenyl-5(2H)-isoxazolone, 9CI. 4-Phenyl-5-isoxazolol, 9CI

[17147-69-2]



$C_9H_7NO_2$ M 161.1
Cryst. (EtOH). Mp 135-137° (131-133°) dec. pK_a 3.50 (25°, H_2O).

NH-form

N-*Benzoyl:* [17147-77-2].
$C_{16}H_{11}NO_3$ M 265.2 Cryst. (EtOH). Mp 161°.

N-*Me:* [7713-60-2]. *2-Methyl-4-phenyl-5(2H)-isoxazolone*
$C_{10}H_9NO_2$ M 175.1 Cryst. (EtOH). Mp 145-147°.

N-*Ph:* [17229-74-2]. *2,4-Diphenyl-5(2H)-isoxazolone*
$C_{15}H_{11}NO_2$ M 237.2 Needles (EtOH). Mp 175° (170.5-172.5°).

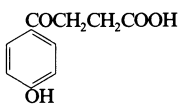
[53485-13-5]

Rupe, H. *et al*, *Helv. Chim. Acta*, 1923, **6**, 102 (*N-Ph*)
De Sarlo, F. *et al*, *Tetrahedron*, 1966, **22**, 2989 (*N-Me*)
Eiden, F. *et al*, *Arch. Pharm. (Weinheim, Ger.)*, 1967, **300**, 615 (*synth, ir*)
De Sarlo, F. *et al*, *J. Het. Chem.*, 1967, **4**, 533 (*synth, uv*)
Maquestiau, A. *et al*, *Org. Magn. Reson.*, 1974, **6**, 224 (*N-15 nmr, tautom*)
Beccalli, E.M. *et al*, *J.O.C.*, 1984, **49**, 4287 (*synth*)
Prager, R.H. *et al*, *Aust. J. Chem.*, 1994, **47**, 1673 (*pmr*)

4-(4-Hydroxyphenyl)-4-oxobutanoic acid H-1-00171

4-Hydroxy-γ-oxobenzenebutanoic acid, 9CI. 3-(4-Hydroxybenzoyl)propanoic acid

[56872-39-0]



$C_{10}H_{10}O_4$ M 194.1

Me ester: [39560-32-2].
$C_{11}H_{12}O_4$ M 208.2 Cryst. (MeOH aq.). Mp 114-117°.

Et ester: [66123-43-1].
$C_{12}H_{14}O_4$ M 222.2 Mp 108-110°.

Nitrile: [7182-43-6]. *4-(4-Hydroxyphenyl)-4-oxobutanenitrile*
$C_{10}H_9NO_2$ M 175.1 Mp 155-157°.

Nitrile, Me ether: [55234-56-5]. *4-(4-Ethoxyphenyl)-4-oxobutanenitrile*
$C_{11}H_{11}NO_2$ M 189.2 Mp 90-92°.

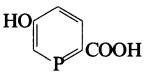
Me ether: [3153-44-4]. *4-(4-Methoxyphenyl)-4-oxobutanoic acid*
$C_{11}H_{12}O_4$ M 208.2 Cryst. (MeOH). Mp 144-145°.

Et ether: [53623-37-3]. *4-(4-Ethoxyphenyl)-4-oxobutanoic acid*
$C_{12}H_{14}O_4$ M 222.2 Needles (C_6H_6). Mp 138-139°.
▶ Irritant.

Gabriel, S. *et al*, *Chem. Ber.*, 1899, **32**, 404 (*Et ether*)
Rao, Y.S. *et al*, *Org. Prep. Proced. Int.*, 1971, **3**, 177 (*Me ether*)
Kuchar, M. *et al*, *Coll. Czech. Chem. Comm.*, 1986, **51**, 2617 (*synth, Me ester, Me ether*)
Dillard, R.D. *et al*, *J. Med. Chem.*, 1991, **34**, 2768 (*Et ester*)

5-Hydroxy-2-phosphorincarboxylic acid, 9CI H-1-00172

[109541-67-5]



$C_6H_5O_3P$ M 156.0
Solid. Mp 172°.

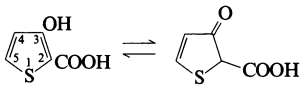
Et ester: [108803-49-2]. *Ethyl 5-hydroxy-2-phosphorincarboxylate*
$C_8H_9O_3P$ M 184.1 Solid. Mp 135°.

Dimethylamide: [109541-69-7]. *5-Hydroxy-N,N-dimethyl-2-phosphorincarboxamide*
$C_8H_{10}NO_2P$ M 183.1 No phys. props. reported.

Pellon, P. *et al*, *Tet. Lett.*, 1986, **27**, 4299, 5611 (*synth, ms, pmr, P-31 nmr*)

3-Hydroxy-2-thiophenecarboxylic acid H-1-00173

3-Oxo-2H-thiophene-2-carboxylic acid



$C_5H_4O_3S$ M 144.1
Plates (Me_2CO). Mp 108°.

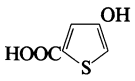
Me ester:
$C_6H_6O_3S$ M 158.1 Prisms (MeOH). Mp 40°. Bp_{13} 108°.

Et ester:
$C_7H_8O_3S$ M 172.2 Liq. Bp_{16} 109°, $Bp_{0.4}$ 63-65°, $Bp_{0.1}$ 73-75°.

O-tert-*Butyl, Et ester:*
$C_{11}H_{16}O_3S$ M 228.3 Liq. $Bp_{0.3}$ 96-98°.

Fiesselmann, H. *et al*, *Chem. Ber.*, 1954, **87**, 841 (*synth*)
Jakobsen, H.J. *et al*, *Tetrahedron*, 1965, **21**, 3331 (*Et ester, synth*)
Hunter, G.A. *et al*, *J.C.S. Perkin 1*, 1995, 1209 (*Et ester synth, pmr, cmr, ms*)

3-Hydroxy-5-thiophenecarboxylic acid H-1-00174



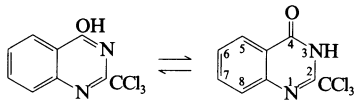
$C_5H_4O_3S$ M 144.1
Plates (C_6H_6/dioxan). Mp 202°.

Fiesselmann, H. *et al*, *Chem. Ber.*, 1954, **87**, 841 (*synth*)

4-Hydroxy-2-(trichloromethyl)quinazoline H-1-00175

2-(Trichloromethyl)-4(1H)-quinazolinone, 9CI. 2-(Trichloromethyl)-4(3H)-quinazolinone

[5558-95-2]



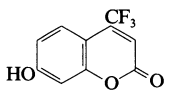
$C_9H_5Cl_3N_2O$ M 263.5
3*H*-form (illus.) prob. in equilib. with 1*H* and *OH*-forms. Cryst. (MeOH). Mp 211-213°.

Samurai, L.I. *et al*, *Zh. Org. Khim.*, 1965, **1**, 2004; *CA*, **64**, 8180b (*synth*)
Holan, G. *et al*, *J.C.S.(C)*, 1967, 20 (*synth, ir, uv*)
Vovk, M.V. *et al*, *Khim. Geterotsikl. Soedin.*, 1991, 698; *CA*, **115**, 279947a (*synth*)

7-Hydroxy-4-(trifluoromethyl)-2*H*-1-benzopyran-2-one, 9CI H-1-00176

7-Hydroxy-4-(trifluoromethyl)coumarin

[575-03-1]



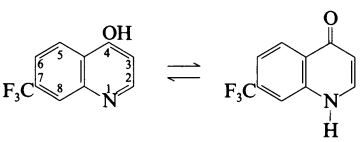
$C_{10}H_5F_3O_3$ M 230.1
Cryst. Mp 184-185°.

Bayer, V. *et al*, *J. Fluorine Chem.*, 1982, **20**, 187 (*synth, pmr, F-19 nmr*)
Pastor, R.E. *et al*, *Can. J. Chem.*, 1987, **65**, 1356 (*cmr*)

4-Hydroxy-7-(trifluoromethyl)quinoline H-1-00177

7-Trifluoromethyl-4(1H)-quinolinone. 7-Trifluoromethyl-4-quinolinol, 9CI

[322-97-4]



$C_{10}H_6F_3NO$ M 213.1
Cryst. (EtOH aq.). Mp 266-269°.

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 860D.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 737D.
Snyder, H.R. *et al*, *J.A.C.S.*, 1947, **69**, 371 (*synth*)
Mooradian, A. *et al*, *J.A.C.S.*, 1949, **71**, 3507 (*synth*)

4-Hydroxy-8-(trifluoromethyl) quinoline H-1-00178

8-Trifluoromethyl-4(1H)-quinolinone. 8-Trifluoromethyl-4-quinolinol, 9CI

[23779-96-6]

$C_{10}H_6F_3NO$ M 213.1
Cryst. (Me_2CO). Mp 180°.

Ger. Pat., 1 815 467, (1969); *CA*, **71**, 91340r (*synth*)
Barlin, G.B. *et al*, *Aust. J. Chem.*, 1992, **46**, 21 (*synth, pmr*)

3-Hydroxy-2,2,4-trimethylpentanal, 9CI H-1-00179

3-Hydroxy-2,2,4-trimethylvaleraldehyde, 8CI. 2,2,4,4-Tetramethylaldol. Isobutyraldol

[918-79-6]

$(H_3C)_2CHCH(OH)C(CH_3)_2CHO$

$C_8H_{16}O_2$ M 144.2

(±)-***form***
Bp_{13} 89-90°, Bp_4 75-77°.

Oxime: [27050-87-9].
$C_8H_{17}NO_2$ M 159.2 $Bp_{0.5}$ 92-95°.

Saunders, R.D. *et al*, *J.A.C.S.*, 1943, **65**, 1714 (*synth*)
Hine, J. *et al*, *J.O.C.*, 1965, **30**, 1184 (*pmr*)
Nakano, T. *et al*, *Synthesis*, 1986, 774 (*synth, cmr*)

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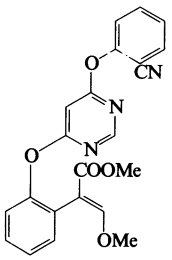
ICI A5504 I-1-00001

Methyl 2-[[6-(2-cyanophenoxy)-4-pyrimidinyl] oxy]-α-(methoxymethylene)benzeneacetate

[131860-33-8]



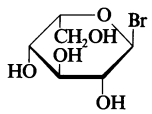
$C_{22}H_{17}N_3O_5$ M 403.3

Fungicide with protectant, systemic and eradicant props.

Eur. Pat., 382 375, (1990); *CA*, **114**, 81870f (*synth*)

Clough, J.M. *et al*, *Chem. Br.*, 1995, 466 (*rev*)

Idopyranosyl bromide I-1-00002



$C_6H_{11}BrO_5$ M 243.0

α-L-form

Tetra-Ac: [14795-18-7].
$C_{14}H_{19}BrO_9$ M 411.2 Cryst. (CH_2Cl_2/Et_2O/pentane). Mp 126-127°. $[\alpha]_D$ −120 (c, 0.75 in $CHCl_3$).

2,3,4-Tribenzoyl, 6-Ac: [117129-63-2].
$C_{29}H_{25}BrO_9$ M 597.4 Syrup.

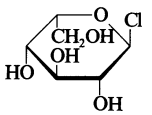
3-Benzyl, tri-Ac: [103703-02-2].
$C_{19}H_{23}BrO_8$ M 459.2 Syrup.

Eur. Pat., 84 999, (1983); *CA*, **100**, 7066t (*tetra-Ac*)

Van Boeckel, C.A.A. *et al*, *J. Carbohydr. Chem.*, 1985, **4**, 293 (*tri-Ac*)

Petitou, M. *et al*, *Tet. Lett.*, 1988, **29**, 1389 (*tribenzoyl*)

Idopyranosyl chloride I-1-00003



$C_6H_{11}ClO_5$ M 198.6

α-L-form

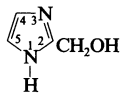
2,3,4-Tribenzyl, 6-(chloroacetyl): [109914-66-1].
$C_{29}H_{30}Cl_2O_6$ M 545.4 Syrup. $[\alpha]_D^{20-24}$ −41 (c, 1 in $CHCl_3$). Unstable at ambient temp.

Jacquinet, J.C. *et al*, *Carbohydr. Res.*, 1987, **159**, 229 (*tribenzyl deriv, pmr*)

1*H*-Imidazole-2-methanol, 9CI I-1-00004

2-(Hydroxymethyl)-1H-imidazole

[3724-26-3]



$C_4H_6N_2O$ M 98.1

Syrup; cryst. (95% EtOH).

Hydrochloride: Needles (EtOH/Et_2O). Mp 111-113°.

Picrate: Yellow needles (EtOH). Mp 151-152°.

N-*Me:* [17334-08-6]. *2-(Hydroxymethyl)-1-methylglyoxaline*
$C_5H_8N_2O$ M 112.1 Cryst. (MeOH). Mp 103-105°.

Jones, R.G., *J.A.C.S.*, 1949, **71**, 383 (*synth*)

Jocelyn, P.C. *et al*, *J.C.S.*, 1957, 3305 (*N-Me*)

Iversen, P.E. *et al*, *Acta Chem. Scand.*, 1966, **20**, 2649 (*N-Me*)

Alley, P.W., *J.O.C.*, 1975, **40**, 1837 (*synth, bibl, pmr*)

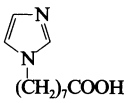
Somayaji, V. *et al*, *J.O.C.*, 1986, **51**, 4866 (*synth, bibl, N-Me*)

Reese, C.B. *et al*, *J.C.S. Perkin 1*, 1993, 2291 (*N-Me, synth, pmr*)

1*H*-Imidazole-1-octanoic acid, 9CI I-1-00005

OKY 025. OKY 1553

[68887-68-3]



$C_{11}H_{18}N_2O_2$ M 210.2

Thromboxane synthetase inhibitor. Antineoplastic agent.

Hydrochloride: [72348-99-3]. Leaflets (EtOH). Mp 153-154°.

Me ester: [72338-73-9].
$C_{12}H_{20}N_2O_2$ M 224.3 Pale yellow oil. $Bp_{1.0}$ 165-170°.

[73031-33-1]

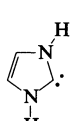
Tanouchi, T. *et al*, *J. Med. Chem.*, 1981, **24**, 1139, 1149 (*synth, ir, pmr, pharmacol*)

Kayama, N. *et al*, *Prostaglandins*, 1981, **21**, 543 (*activity*)

Butler, K.D. *et al*, *Thromb. Haemostasis*, 1982, **47**, 46 (*pharmacol*)

Groves, J.T. *et al*, *J.A.C.S.*, 1989, **111**, 2900 (*synth, pmr*)

2-Imidazolylidene I-1-00006



$C_3H_4N_2$ M 68.0

N,N′-*Di-Me:* [52356-52-2]. *1,3-Dihydro-1,3-dimethyl-2H-imidazol-2-ylidene, 9CI*

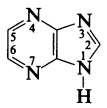
$C_5H_8N_2$ M 96.1 Simple isolable carbene. Liq. Stable several days in soln., neat liq. rapidly dec.

N,N′-*Di-1-adamantyl:*
$C_{23}H_{32}N_2$ M 336.5 First authenticated stable carbene. Prisms (toluene). Mp 240-241°. Melts undec. Stable in absence of air and moisture.

Arduengo, A.J. *et al*, *J.A.C.S.*, 1991, **113**, 361; 1992, **114**, 5530 (*synth, pmr, cmr, cryst struct*)

1*H*-Imidazo[4,5-*b*]pyrazine, 9CI I-1-00007

[273-94-9]



$C_5H_4N_4$ M 120.1

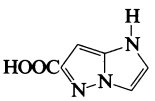
Cryst. (H_2O). Mp 258-259°.

Muehlmann, F.L. *et al*, *J.A.C.S.*, 1956, **78**, 242 (*synth*)

Sharma, R.A. *et al*, *J. Med. Chem.*, 1973, **16**, 643 (*synth, pmr*)

1*H*-Imidazo[1,2-*b*]pyrazole-6-carboxylic acid I-1-00008

[159181-78-9]



$C_6H_5N_3O_2$ M 151.1

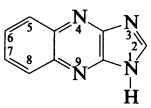
Solid. Mp 230° dec.

Et ester:
$C_8H_9N_3O_2$ M 179.1 Cryst. (EtOAc/hexane). Mp 160°.

Vanotti, E. *et al*, *J. Het. Chem.*, 1994, **31**, 737.

1*H*-Imidazo[4,5-*b*]quinoxaline I-1-00009

[269-81-8]



$C_9H_6N_4$ M 170.1

Cryst. (AcOH). Mp 286°.

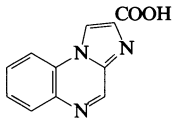
Schipper, E. *et al*, *J.A.C.S.*, 1951, **73**, 5672 (*synth, uv*)

Obafemi, C.A. *et al*, *Helv. Chim. Acta*, 1994, **77**, 1549 (*synth, uv, pmr*)

Imidazo[1,2-*a*]quinoxaline-2-carboxylic acid, 9CI I-1-00010

Dazoquinast, INN

[76002-75-0]



$C_{11}H_7N_3O_2$ M 213.1

Antiallergic agent. Cryst. (EtOH aq.). Mp 274-275°.

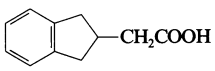
[76013-27-9]

Ager, I.R. *et al, J. Med. Chem.*, 1988, **31**, 1098 (*synth, pharmacol*)

2-Indaneacetic acid I-1-00011

2,3-Dihydro-1H-indene-2-acetic acid, 9CI

[37868-26-1]



$C_{11}H_{12}O_2$ M 176.2

Cryst. (EtOH aq.). Mp 88-90°. $Bp_{0.8}$ 142-144°.

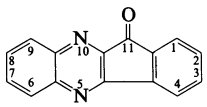
Me ester: [53273-37-3].
$C_{12}H_{14}O_2$ M 190.2 Liq. $Bp_{0.7}$ 90°. $n_D^{26.5}$ 1.5168.

Chloride: [18691-34-4].
$C_{11}H_{11}ClO$ M 194.6 Oil. Bp_3 115-116°.

Bergmann, E.D. *et al, J.O.C.*, 1961, **26**, 3555 (*ester*)
Tanaka, Y. *et al, J. Med. Chem.*, 1994, **37**, 2071 (*synth, ir, pmr*)

11*H*-Indeno[1,2-*b*]quinoxalin-11-one, 9CI I-1-00012

[6954-91-2]



$C_{15}H_8N_2O$ M 232.2

Yellow needles (MeOH or EtOH). Mp 220-221° (217-219°).

Oxime: [23146-22-7].
$C_{15}H_9N_3O$ M 247.2 Needles (EtOH aq.). Mp 257°.

5-Oxide: [6965-50-0].
$C_{15}H_8N_2O_2$ M 248.2 Orange needles (C_6H_6). Mp 275° dec. (268-271° dec.).

6,7,8,9-Tetrahydro: [124942-09-2].
$C_{15}H_{12}N_2O$ M 236.2 Yellow needles (EtOAc). Mp 178-182°.

6,7,8,9-Tetrahydro, 5-oxide:
$C_{15}H_{12}N_2O_2$ M 252.2 Yellow needles (DMSO). Mp 237-239°.

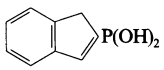
6,7,8,9-Tetrahydro, 10-oxide:
$C_{15}H_{12}N_2O_2$ M 252.2 Yellow needles (DMSO). Mp 269-271°.

6,7,8,9-Tetrahydro, 5,10-dioxide:
$C_{15}H_{12}N_2O_3$ M 268.2 Dark red prisms (EtOAc). Mp 193-195°.

Pfeiffer, P. *et al, Ber.*, 1938, **71**, 272 (*synth*)
Pearson, B.D. *et al, J.O.C.*, 1962, **27**, 1674 (*synth, oxime, 5-oxide, uv, ir*)
Schönberg, A. *et al, Chem. Ber.*, 1977, **110**, 3954 (*uv, ir, cmr, ms*)
Deady, L.W. *et al, Tetrahedron*, 1993, **49**, 9823 (*pmr, 5-oxide*)
Mazhukin, D.G. *et al, Annalen*, 1994, 983 (*tetrahydro*)

2-Indenylphosphonous acid, 9CI I-1-00013

2-Indenephosphonous acid



$C_9H_9O_2P$ M 180.1

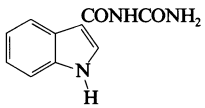
Dichloride: [85741-86-2].
$C_9H_7Cl_2P$ M 217.0 Liq. Bp_2 120-121°.

Timokhin, B.V. *et al, Zh. Obshch. Khim.*, 1983, **53**, 291; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1983, **53**, 252 (*synth, P-31 nmr*)

***N*-(1*H*-Indole-3-carbonyl)urea** I-1-00014

N-(Aminocarbonyl)-1H-indole-3-carboxamide, 9CI

[159308-53-9]



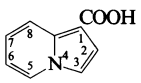
$C_{10}H_9N_3O_2$ M 203.2

Metab. from the sponge *Zyzza massalis.*

Mancini, I. *et al, Helv. Chim. Acta*, 1994, **77**, 1886 (*isol, uv, pmr, cmr, ms, struct*)

1-Indolizinecarboxylic acid, 9CI I-1-00015

[90347-97-0]



$C_9H_7NO_2$ M 161.1

Needles (EtOH). Mp 184-185° dec.

Et ester:
$C_{11}H_{11}NO_2$ M 189.2 Pale yellow oil. Bp_3 124°. Shows intense blue fluorescence in EtOH.

Amide: [14759-47-8].
$C_9H_8N_2O$ M 160.1 Needles (C_6H_6/EtOH). Mp 148-149°.

Nitrile: 1-Cyanoindolizine
$C_9H_6N_2$ M 142.1 Needles (petrol). Mp 52-53°.

Bragg, D.R. *et al, J.C.S.*, 1963, 3277 (*synth*)
Hurst, J. *et al, J.C.S.*, 1965, 2948 (*synth, ir, nitrile*)
Melton, T. *et al, J.C.S.(C)*, 1967, 983 (*synth, ir, amide*)

2-Indolizinecarboxylic acid, 9CI I-1-00016

Pyrrolo[1,2-a]pyridine-2-carboxylic acid. 2-Pyrrocolinecarboxylic acid (obsol.)

[3189-48-8]

$C_9H_7NO_2$ M 161.1

Small buff needles or cubes (EtOH). Mp 240-241° dec.

Me ester: [16959-62-9].
$C_{10}H_9NO_2$ M 175.1 Platelets (EtOH aq.); cryst. (hexane). Mp 97-99°.

Amide: [22320-23-6].
$C_9H_8N_2O$ M 160.1 Cryst. (H_2O). Mp 158°.

Nitrile: [153274-67-0]. *2-Cyanoindolizine*
$C_9H_6N_2$ M 142.1 Cryst. (hexane). Mp 67.5-69°.

Diels, O. *et al, Annalen*, 1932, **498**, 16 (*synth*)
Borrows, E.T. *et al, J.C.S.*, 1947, 672 (*synth*)
Wiley, R.H. *et al, J.O.C.*, 1953, **18**, 836 (*synth*)
Jones, G. *et al, J.C.S.(C)*, 1969, 901 (*amide, ester*)
Bode, M.L. *et al, J.C.S. Perkin 1*, 1990, 1612; 1993, 1809; 1994, 3023 (*deriv, synth, ir, pmr, cmr*)

3-Indolizinecarboxylic acid, 9CI I-1-00017

$C_9H_7NO_2$ M 161.1

Me ester: [22320-25-8].
$C_{10}H_9NO_2$ M 175.1 Liq. Bp_{14} 144-146°.

Chloride: [22380-17-2].
C_9H_6ClNO M 179.6 Cryst. (petrol). Mp 82°.

Amide: [22320-27-0].
$C_9H_8N_2O$ M 160.1 Cryst. (EtOAc). Mp 146-147°.

Nitrile: [72090-73-4]. *3-Cyanoindolizine*
$C_9H_6N_2$ M 142.1 Cryst. Mp 46-48°.

[55814-14-7]

Jones, G. *et al, J.C.S.(C)*, 1969, 901 (*synth, ir, pmr, derivs*)
Matsumoto, K. *et al, Synthesis*, 1979, 746 (*synth, nitrile*)

8-Indolizinecarboxylic acid I-1-00018

$C_9H_7NO_2$ M 161.1

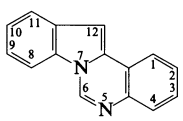
Nitrile: [52951-21-0]. *8-Cyanoindolizine*
$C_9H_6N_2$ M 142.1 Fine, lemon-yellow needles with a penetrating odour. Mp 74-75°.

[71081-71-5]

Jutz, C. *et al, Angew. Chem., Int. Ed.*, 1974, **13**, 737 (*synth, pmr, uv, nitrile*)

Indolo[1,2-*c*]quinazoline, 9CI I-1-00019

[239-43-0]



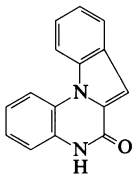
$C_{15}H_{10}N_2$ M 218.2

Cryst. (EtOH). Mp 201°.

Kiang, A.K. *et al, J.C.S.*, 1956, 1319 (*synth*)
Billimoria, A.D. *et al, J.O.C.*, 1994, **59**, 6777 (*synth, pmr, ms*)

Indolo[1,2-*a*]quinoxalin-6(5*H*)-one I-1-00020

6-Hydroxyindolo[1,2-a]quinoxaline. Indolo[1,2-a]quinoxalin-6-ol



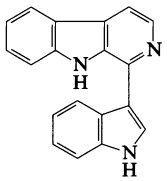
$C_{15}H_{10}N_2O$ M 234.2
Beige solid (DMF). Mp >300°.

Beach, M.J. *et al*, *Synth. Commun.*, 1995, **25**, 2165 (*synth, ir, pmr*)

1-(3-Indolyl)-β-carboline I-1-00021

1-(1H-Indol-3-yl)-9H-pyrido[3,4-b]indole, 9CI. ***Eudistomin U***

[155885-64-6]



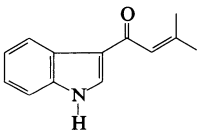
$C_{19}H_{13}N_3$ M 283.3
Alkaloid from the Caribbean ascidian *Lissoclinum fragile*. Exhibits antibacterial activity. Yellow foam.

Badre, A. *et al*, *J. Nat. Prod.*, 1994, **57**, 528 (*isol, uv, ir, pmr, cmr, ms, struct*)

1-(1*H*-Indol-3-yl)-3-methyl-2-buten-1-one, 9CI I-1-00022

3-(3-Methyl-1-oxo-2-butenyl)-1H-indole

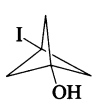
[50615-00-4]



$C_{13}H_{13}NO$ M 199.2
Alkaloid from root bark of *Pamburus missionis* (Rutaceae). Needles (CH_2Cl_2/hexane). Mp 136.5-138° (130-131°).

Somei, M. *et al*, *Tet. Lett.*, 1973, 2451 (*synth*)
Wenkert, E. *et al*, *J.O.C.*, 1986, **51**, 2343 (*synth*)
Kumar, V. *et al*, *Phytochemistry*, 1994, **36**, 879 (*isol, uv, ir, pmr, cmr, ms*)

3-Iodobicyclo[1.1.1]pentan-1-ol I-1-00023



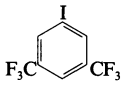
C_5H_7IO M 210.0

Me ether: [136863-37-1]. *1-Iodo-3-methoxybicyclo[1.1.1]pentane*
C_6H_9IO M 224.0 No phys. props. descr.

Wiberg, K.B. *et al*, *J.A.C.S.*, 1991, **113**, 8995.
Della, E.W. *et al*, *J.O.C.*, 1994, **59**, 2986 (*Me ether, synth, pmr*)

1-Iodo-3,5-bis(trifluoromethyl) benzene, 9CI I-1-00024

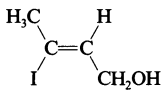
[328-73-4]



$C_8H_3F_6I$ M 340.0
Oil. d 1.92. Bp_{10} 59-61°.

Ross, S.D. *et al*, *J.A.C.S.*, 1953, **75**, 4967 (*synth*)
Fujiki, K. *et al*, *J. Fluorine Chem.*, 1992, **57**, 307 (*synth*)

3-Iodo-2-buten-1-ol I-1-00025



C_4H_7IO M 198.0

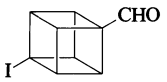
(Z)-form
Oil.

Beruben, D. *et al*, *J.O.C.*, 1995, **60**, 2488 (*synth, pmr, cmr*)

4-Iodo-1-cubanecarboxaldehyde I-1-00026

4-Iodopentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octanecarboxaldehyde, 9CI. 1-Formyl-4-iodocubane

[163332-88-5]

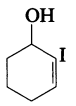


C_9H_7IO M 258.0
Cryst. (hexane). Mp >130° dec.

Eaton, P.E. *et al*, *J.A.C.S.*, 1994, **116**, 7588 (*synth, pmr, cmr*)

2-Iodo-2-cyclohexen-1-ol I-1-00027

[155791-58-5]



C_6H_9IO M 224.0

(±)-form
Cubes (Et_2O/petrol). Mp 44-45°.

Adam, W. *et al*, *J.O.C.*, 1994, **59**, 2695 (*synth, pmr, cmr, ir*)

10-Iododecanal I-1-00028

[148019-71-0]

$ICH_2(CH_2)_8CHO$

$C_{10}H_{19}IO$ M 282.1
Liq.

Burger, A. *et al*, *J. Med. Chem.*, 1993, **36**, 1418 (*synth, pmr, ms*)

10-Iodo-1-decanol I-1-00029

[57395-49-0]

$ICH_2(CH_2)_8CH_2OH$

$C_{10}H_{21}IO$ M 284.1
Cryst. (pentane at −20°). Mp 26-27°.

Biogegrain, R. *et al*, *Tet. Lett.*, 1975, 2529 (*synth*)
Burger, A. *et al*, *J. Med. Chem.*, 1993, **36**, 1418 (*synth, pmr, ms*)

1-Iodo-1-decyne, 9CI I-1-00030

Iodo(octyl)acetylene

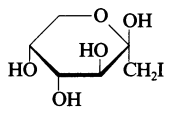
[67826-81-7]

$H_3C(CH_2)_7C{\equiv}CI$

$C_{10}H_{17}I$ M 264.1
Pale yellow oil. $Bp_{0.7}$ 84°. $n_D^{23.6}$ 1.4987.

Vaughn, T.H., *J.A.C.S.*, 1933, **55**, 3453 (*synth*)
Ochiai, M. *et al*, *J.O.C.*, 1989, **54**, 4038 (*pmr, cmr, ms*)
Lando, J.B. *et al*, *Chem. Mater.*, 1994, **6**, 1444 (*synth, pmr*)
Rao, M.L.N. *et al*, *Synth. Commun.*, 1995, **25**, 2295 (*synth, cmr*)

1-Iodo-1-deoxyfructose I-1-00031



β-D-Pyranose-*form*

$C_6H_{11}IO_5$ M 290.0

D-form

Tetra-Ac:
$C_{14}H_{19}IO_9$ M 458.2 Mp 55-56°. $[\alpha]_D$ +63 ($CHCl_3$).

β-D-Pyranose-form

3,4,5-Tribenzoyl: [134136-51-9].
$C_{27}H_{23}IO_8$ M 602.3 Syrup.

2,3:4,5-Di-O-isopropylidene: [38084-03-6].
$C_{12}H_{19}IO_5$ M 370.1 Oil. $[\alpha]_D^{24}$ −21.4 (c, 4.5 in $CHCl_3$).

Wolfrom, M.L. *et al*, *J.A.C.S.*, 1943, **65**, 1516 (D-tetra-Ac)
James, K. *et al*, *Aust. J. Chem.*, 1972, **25**, 1967 (*diisopropylidene, pmr*)
Campbell, M.H. *et al*, *Tet. Lett.*, 1991, **32**, 1237 (*tribenzoyl*)

1-Iodo-3,3-dimethyl-1-butene, 9CI I-1-00032

[159217-27-3]

$(H_3C)_3CCH{=}CHI$

$C_6H_{11}I$ M 210.0

(E)-form [61382-45-4]
Liq. Bp_{59} 70-72°.

(Z)-form [64245-24-5]
Liq. Bp_{65} 70-72°. n_D^{25} 1.5008.

Miller, R.B. *et al*, *J.O.C.*, 1978, **43**, 4424 (*synth, ir, pmr*)
Brown, H.C. *et al*, *J.O.C.*, 1989, **54**, 6064, 6068, 6075 (*synth, cmr, pmr*)
Kiehl, A. *et al*, *Annalen*, 1995, 223 (*synth, cmr, pmr*)

6-Iodo-5,5-dimethyl-1-hexene, 9CI I-1-00033

[77400-57-8]

$H_2C{=}CHCH_2CH_2C(CH_3)_2CH_2I$

$C_8H_{15}I$ M 238.1
Liq. $Bp_{1.5}$ 46°. n_D^{25} 1.5020.

Ashby, E.C. *et al*, *J.O.C.*, 1984, **49**, 3545 (*synth, pmr, ms*)

4-Iodo-2(5*H*)-furanone, 9CI I-1-00034

[155140-39-9]

$C_4H_3IO_2$ M 209.9
Cryst. Mp 101-102°.

Sweeney, J.B. *et al*, *Synth. Commun.*, 1994, **24**, 755 (*synth, ir, pmr, cmr, ms*)

1-Iodo-1-heptyne, 9CI I-1-00035

Amyliodoacetylene. Iodo(pentyl)acetylene

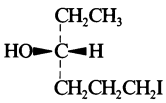
[54573-13-6]

$H_3C(CH_2)_4C{\equiv}CI$

$C_7H_{11}I$ M 222.0
Liq. d^{22} 1.472. Mp −35°. Bp_{21} 93°. n_D^{20} 1.5125.

Vaughn, T.H. *et al*, *J.A.C.S.*, 1933, **55**, 2150 (*synth*)
Murray, M.J. *et al*, *J. Chem. Phys.*, 1944, **12**, 156 (*Raman*)
Ravid, U. *et al*, *Tetrahedron*, 1978, **34**, 1449 (*synth, pmr*)
Bhanu, S. *et al*, *J.C.S. Perkin 1*, 1979, 1218 (*synth*)
Bonnet, B. *et al*, *Synthesis*, 1993, 1071 (*synth, pmr, cmr, ms*)
Rao, M.L.N. *et al*, *Synth. Commun.*, 1995, **25**, 2295 (*synth, cmr*)

6-Iodo-3-hexanol, 9CI I-1-00036



$C_6H_{13}IO$ M 228.0

(*R*)-*form* [161458-59-9]
Reddish liq. Bp_1 120°. $[\alpha]_D^{34}$ −9.7 (c, 1.12 in $CHCl_3$).

Ac:
$C_8H_{15}IO_2$ M 270.1 Liq. Bp_1 118°. $[\alpha]_D^{27}$ +9.8 (c, 3.69 in $CHCl_3$).

Paolucci, C. *et al*, *J.O.C.*, 1995, **60**, 169 (*synth, pmr, cmr*)

6-Iodo-2-hexyne, 9CI I-1-00037

[28077-74-9]

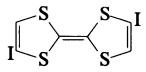
$H_3CC{\equiv}CCH_2CH_2CH_2I$

C_6H_9I M 208.0
Liq. Bp_{35} 99-104°.

Peterson, P.E. *et al*, *J.A.C.S.*, 1970, **92**, 2834 (*synth*)
Anderson, B.A. *et al*, *J.A.C.S.*, 1993, **115**, 10671 (*synth, pmr, cmr, ir, ms*)

4-Iodo-2-(4-iodo-1,3-dithiol-2-ylidene)-1,3-dithiole I-1-00038

2,6(7)-Diiodotetrathiafulvalene. 2,2′-Bi(4-iodo-1,3-dithiol-2-ylidene)



$C_6H_2I_2S_4$ M 456.1

(*E*)-*form* [121108-19-8]
Orange plates (CS_2/petrol). Mp 100° dec. Dec. *ca.* 130°.

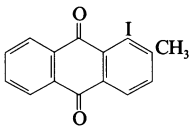
[121108-11-0]

Kreitsberga, Ya.N. *et al*, *Zh. Org. Khim.*, 1989, **25**, 1456; *J. Org. Chem. USSR* (*Engl. Transl.*), 1989, **25**, 1312 (*synth*)
Wang, C. *et al*, *Chem. Comm.*, 1994, 983 (*synth, pmr, cmr, cryst struct*)

1-Iodo-2-methylanthraquinone I-1-00039

1-Iodo-2-methyl-9,10-anthracenedione, 9CI

[74214-82-7]



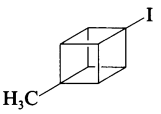
$C_{15}H_9IO_2$ M 348.1
Cryst. Mp 169-171°.

Scholl, R. *et al*, *Ber.*, 1907, **40**, 1696 (*synth*)
Kim, J.I. *et al*, *J.A.C.S.*, 1992, **114**, 9309 (*synth, pmr*)

1-Iodo-4-methylcubane I-1-00040

4-Methylcubyl iodide. 1-Iodo-4-methylpentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane, 9CI

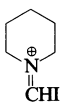
[125762-85-8]



C_9H_9I M 244.0
Cryst. powder. Mp 79-81°.

Eaton, P.E. *et al*, *J.O.C.*, 1995, **60**, 966 (*synth, pmr, cmr*)

N-(Iodomethylene) piperidinium(1+) I-1-00041



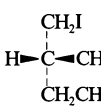
$C_6H_{11}IN^{\oplus}$ M 224.0 (ion)

Iodide:
$C_6H_{11}I_2N$ M 350.9 Yellow needles.

Weiss, R. *et al*, *Angew. Chem., Int. Ed.*, 1994, **33**, 893 (*synth, ir, pmr, cmr, cryst struct*)

1-Iodo-2-methylpentane I-1-00042

[31294-94-7]



(*R*)-*form*

$C_6H_{13}I$ M 212.0

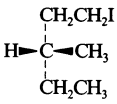
(*R*)-*form* [18450-71-0]
Liq. Bp 162-166°. $[\alpha]_D^{21}$ −0.68 (c, 6.6 in MeOH). n_D^{19} 1.4941.

(*S*)-*form*
Liq. Bp_{50} 83-85°. $[\alpha]_D^{21}$ +0.68 (c, 6.87 in MeOH).

Mori, K. *et al*, *Annalen*, 1994, 1153 (*synth, ir, pmr*)

1-Iodo-3-methylpentane, 9CI I-1-00043

[24346-53-0]



(*R*)-*form*

$C_6H_{13}I$ M 212.0

(*R*)-*form*
Liq. Bp_{12} 54°. $[\alpha]_D^{25}$ −7.61 (neat). n_D^{25} 1.4866.

(±)-*form*
Liq. Bp_{30} 72-75°.

Levene, P.A. *et al*, *J. Biol. Chem.*, 1936, **115**, 415 (*R-form*)
Suzuki, T. *et al*, *Agric. Biol. Chem.*, 1981, **45**, 1357 (*synth, ir*)

Iodomethylpropanedioic acid, 9CI I-1-00044

Iodomethylmalonic acid

[69858-37-3]

$HOOCC(CH_3)ICOOH$

$C_4H_5IO_4$ M 243.9
Prepd. *in situ*; not isol.

Dinitrile: [138976-63-3]. *Iodomethyl propanedinitrile, 9CI. Dicyanoiodomethane*
$C_4H_3IN_2$ M 205.9 Oil which cryst. at 0°.

Furrow, S.D., *Int. J. Chem. Kinet.*, 1979, **11**, 131 (*synth, uv*)
Thoma, G. *et al*, *J.A.C.S.*, 1993, **115**, 8585 (*dinitrile*)

(Iodomethyl) triphenylphosphonium(1+) I-1-00045

$Ph_3P^{\oplus}CH_2I$

$C_{19}H_{17}IP^{\oplus}$ M 403.2 (ion)

Iodide: [3020-28-8].
$C_{19}H_{17}I_2P$ M 530.1 Needles. Mp 240° dec.

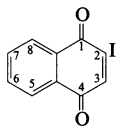
[98822-67-4, 110428-39-2]

Scherfise, K.D. *et al*, *Z. Naturforsch., B*, 1985, **40**, 906 (*synth, ir, cryst struct*)
Stahl, K. *et al*, *J. Organomet. Chem.*, 1986, **316**, 85 (*synth*)
Li, S. *et al*, *Chem. Ber.*, 1990, **123**, 1441 (*use*)
Vogt, H. *et al*, *Z. Naturforsch., B*, 1993, **48**, 1760 (*synth, ms, P-31 nmr, cryst struct*)
Lauritsen, K. *et al*, *Z. Anorg. Allg. Chem.*, 1994, **620**, 1103 (*iodide, P-31 nmr, reactions*)

2-Iodo-1,4-naphthoquinone, 8CI I-1-00046

2-Iodo-1,4-naphthalenedione, 9CI

[35079-24-4]



$C_{10}H_5IO_2$ M 284.0
Yellow needles (EtOH). Mp 120°.

Hodgson, H. *et al, J.C.S.*, 1935, 1850 (*synth*)
Gaultier, J. *et al, C. R. Hebd. Seances Acad. Sci. Ser. C*, 1971, **273**, 956 (*cryst struct*)
Sharma, J. *et al, Org. Prep. Proced. Int.*, 1995, **27**, 84 (*synth, pmr, uv, ir*)

5-Iodo-1,4-naphthoquinone, 8CI I-1-00047

5-Iodo-1,4-naphthalenedione, 9CI

[62784-50-3]

$C_{10}H_5IO_2$ M 284.0
Red prisms (C_6H_6/hexane). Mp 173-175°.

Ishii, H. *et al, Tetrahedron*, 1976, **32**, 2693 (*synth, ir, uv, pmr*)

6-Iodo-1,4-naphthoquinone, 8CI I-1-00048

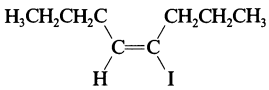
6-Iodo-1,4-naphthalenedione, 9CI

[115782-79-1]

$C_{10}H_5IO_2$ M 284.0
Solid (C_6H_6/hexane). Mp 123-124°.

Shvartsberg, M.S. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1988, 485; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1988, 404 (*synth, pmr*)

4-Iodo-4-octene I-1-00049



(*E*)-*form*

$C_8H_{15}I$ M 238.1

(*E*)-***form*** [81793-05-7]
cis-*form*
Liq.

(*Z*)-***form*** [86223-33-8]
trans-*form*
Liq.

Staley, S.W. *et al, Chem. Comm.*, 1969, 288.
Hudrlik, P.F. *et al, Tetrahedron*, 1983, **39**, 877.
Kropp, P.J. *et al, J.O.C.*, 1994, **59**, 3102 (*synth, pmr*)

8-Iodo-1-octene, 9CI I-1-00050

[38380-55-1]

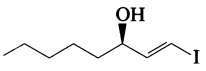
$H_2C{=}CH(CH_2)_5CH_2I$

$C_8H_{15}I$ M 238.1
Liq. Bp_{45} 126-128°, $Bp_{0.2}$ 44-46°.

Sih, C.J. *et al, J.A.C.S.*, 1975, **97**, 857 (*synth, ir, pmr*)
Garanti, L. *et al, Gazz. Chim. Ital.*, 1976, **106**, 187 (*synth*)
Johnson, D.K. *et al, Synth. Commun.*, 1994, **24**, 1557 (*synth, pmr*)

1-Iodo-1-octen-3-ol, 9CI I-1-00051

[73961-62-3]



(*R*)-(*E*)-*form*

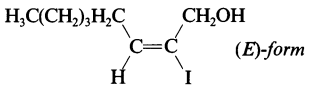
$C_8H_{15}IO$ M 254.1

(*R*)-(*E*)-***form*** [42541-99-1]
$[\alpha]_D^{25}$ −9.9 (c, 1.5 in MeOH).

(*S*)-(*E*)-***form*** [39647-93-3]
Intermed. for synthesis of prostaglandins. Oil. $[\alpha]_D^{24}$ +9.9 (c, 1.6 in MeOH) (100% op).

Kluge, A.F. *et al, J.A.C.S.*, 1972, **94**, 7827 (*synth, resoln, pmr, ir*)
Sih, C.J. *et al, J.A.C.S.*, 1975, **97**, 865 (*synth*)
Jung, M.E. *et al, Tet. Lett.*, 1982, **23**, 3851 (*synth, pmr*)
Noyori, R. *et al, J.A.C.S.*, 1984, **106**, 6717 (*synth, ir, pmr*)
Luo, F.-T. *et al, J.O.C.*, 1985, **50**, 4762 (*synth, pmr, cmr*)
Kitano, Y. *et al, Tet. Lett.*, 1987, **28**, 6351 (*resoln*)
Chemin, D. *et al, Synthesis*, 1993, 377 (*synth, resoln, pmr, cmr*)

2-Iodo-2-octen-1-ol, 9CI I-1-00052



(*E*)-*form*

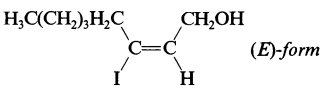
$C_8H_{15}IO$ M 254.1

(*E*)-***form*** [161530-86-5]
Oil.

(*Z*)-***form*** [79970-59-5]
Oil.

Ensley, H.E. *et al, J.O.C.*, 1982, **47**, 404 (*pmr, cmr*)
Zoretic, P.A. *et al, Synth. Commun.*, 1985, **15**, 367 (*pmr*)
Piers, E. *et al, Synthesis*, 1995, 47 (*synth, pmr, cmr, ir*)

3-Iodo-2-octen-1-ol, 9CI I-1-00053



(*E*)-*form*

$C_8H_{15}IO$ M 254.1

(*E*)-***form*** [161530-87-6]
Oil.

(*Z*)-***form*** [63093-31-2]
Oil. $Bp_{0.05}$ 108°.

Duboudin, J.G. *et al, J. Organomet. Chem.*, 1979, **168**, 227 (*synth, pmr*)
Piers, E. *et al, Synthesis*, 1995, 47 (*synth, pmr, cmr, ir*)

1-Iodo-1-pentadecyne, 9CI I-1-00054

[78076-36-5]

$H_3C(CH_2)_{12}C{\equiv}CI$

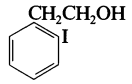
$C_{15}H_{27}I$ M 334.2
Amber liq. Unstable at r.t. and in light.

Holtzapple, M.T. *et al, Org. Prep. Proced. Int.*, 1995, **27**, 507 (*synth, pmr*)

2-(2-Iodophenyl)ethanol I-1-00055

2-Iodobenzeneethanol, 9CI. o-Iodophenethyl alcohol, 8CI

[26059-40-5]



C_8H_9IO M 248.0
Oil. Bp_4 136°. n_D^{25} 1.6154.

Ac: [57527-00-1].
$C_{10}H_{11}IO_2$ M 290.1 Liq. $Bp_{0.01}$ 55°.

Bennett, G.M. *et al, J.C.S.*, 1941, 652 (*synth*)
Acheson, R.M. *et al, J.C.S. Perkin 1*, 1987, 2321 (*synth, ms, ir, pmr*)

2-(3-Iodophenyl)ethanol I-1-00056

3-Iodobenzeneethanol, 9CI

[127201-31-4]

C_8H_9IO M 248.0
Oil.

Van Dort, M.E. *et al, Appl. Radiat. Isot.*, 1992, **43**, 671 (*synth, pmr, ms*)

2-(4-Iodophenyl)ethanol I-1-00057

4-Iodobenzeneethanol, 9CI. p-Iodophenethyl alcohol, 8CI

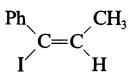
[52914-23-5]

C_8H_9IO M 248.0
Cryst. (Et_2O/hexane). Mp 48-49°. $Bp_{0.5}$ 110-120°.

Bennett, G.M. *et al, J.C.S.*, 1935, 1819; 1941, 652 (*synth*)
Newton, B.N., *J. Med. Chem.*, 1976, **19**, 1362 (*synth, pmr*)
Göbel, M.W. *et al, Annalen*, 1994, 1075 (*synth, ir*)

1-Iodo-1-phenylpropene I-1-00058

(1-Iodo-1-propenyl)benzene, 9CI. α-Iodo-β-methylstyrene. α-Iodopropenylbenzene



C_9H_9I M 244.0

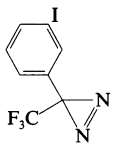
(*E*)-***form*** [32780-80-6]
Obt. by irradiation of (*Z*)-form. Yellow liq. $Bp_{0.3}$ 63-68°.

(*Z*)-***form*** [32780-79-3]
Liq. $Bp_{0.3}$ 64-68°.

Campbell, J.R. *et al, Aust. J. Chem.*, 1971, **24**, 1425 (*synth, uv, ir, pmr*)
Kropp, P.J. *et al, J.O.C.*, 1994, **59**, 3102 (*synth, pmr*)

3-(3-Iodophenyl)-3-(trifluoromethyl)diazirene I-1-00059

[79684-41-6]

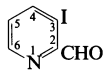


$C_8H_4F_3IN_2$ M 312.0
Photoactivatable probe used for hydrophobic labelling of membrane proteins. Slightly yellow solid.

Brunner, J., *Biochemistry*, 1981, **20**, 7174 (*synth, uv*)
Brunner, J., *Methods Enzymol.*, 1989, **172**, 628 (*bibl*)
White, B.H. *et al*, *J. Biol. Chem.*, 1991, **267**, 15770 (*props*)

3-Iodo-2-pyridinecarboxaldehyde I-1-00060

3-Iodo-2-formylpyridine



C_6H_4INO M 233.0
Cryst. Mp 58-60°.

Björk, P. *et al*, *J. Het. Chem.*, 1995, **32**, 751 (*synth, pmr, ms*)

4-Iodo-3-pyridinecarboxaldehyde I-1-00061

4-Iodo-3-formylpyridine

C_6H_4INO M 233.0
Cryst. Mp 91-92°.

Björk, P. *et al*, *J. Het. Chem.*, 1995, **32**, 751 (*synth, pmr, ms*)

1-Iodo-2-(trifluoromethyl) benzene, 9CI I-1-00062

2-Iodobenzotrifluoride. α,α,α-Trifluoro-o-iodotoluene, 8CI

[444-29-1]

$C_7H_4F_3I$ M 272.0
d 1.94. Bp 197-198°. n_D^{20} 1.53.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 914A.
Aldrich Library of NMR Spectra, 2nd edn., **1**, 784C.
Jones, R.G., *J.A.C.S.*, 1947, **69**, 2346 (*synth*)
Yoder, C.H. *et al*, *J.O.C.*, 1976, **41**, 1511 (*cmr*)
Takagi, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 3691 (*synth*)
Naumann, D. *et al*, *J. Fluorine Chem.*, 1990, **47**, 283 (*synth, F-19 nmr*)

1-Iodo-3-(trifluoromethyl) benzene, 9CI I-1-00063

3-Iodo-α,α,α,α-trifluorotoluene. 3-Iodobenzotrifluoride. α,α,α-Trifluoro-m-iodotoluene, 8CI

[401-81-0]

$C_7H_4F_3I$ M 272.0
Yellow liq. d 1.89. Bp 182-183°, Bp_{25} 82°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 916B.
Finger, G.C. *et al*, *CA*, 1945, **39**, 1146 (*synth*)
Glennon, R.A. *et al*, *J. Med. Chem.*, 1981, **24**, 678 (*synth*)
Naumann, D. *et al*, *J. Fluorine Chem.*, 1990, **47**, 283 (*synth, F-19 nmr*)

1-Iodo-4-(trifluoromethyl) benzene I-1-00064

4-Iodo-α,α,α,α-trifluorotoluene. 4-Iodobenzotrifluoride. α,α,α-Trifluoro-p-iodotoluene, 8CI

[455-13-0]

$C_7H_4F_3I$ M 272.0
d 1.85. Mp 17-17.5°. Bp 185.5-186°.

[100784-66-5]

Jones, R.G., *J.A.C.S.*, 1947, **69**, 2346 (*synth*)
Naumann, D. *et al*, *J. Fluorine Chem.*, 1990, **47**, 283 (*synth, F-19 nmr*)

Iodo(triphenylphosphoranylidene)acetic acid I-1-00065

$Ph_3P{=}CICOOH$

$C_{20}H_{16}IO_2P$ M 446.2
Esters are Wittig reagents.

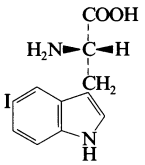
Me ester: [26480-86-4]. *Methyl iodo(triphenylphosphoranylidene)acetate*
$C_{21}H_{18}IO_2P$ M 460.2 Cryst. (EtOH aq.). Mp 165.5-166°.

Et ester: [26480-87-5]. *Ethyl iodo(triphenylphosphoranylidene)acetate*
$C_{22}H_{20}IO_2P$ M 474.2 Cryst. (EtOH aq.). Mp 134-135°.

Sherchuk, M.I. *et al*, *Zh. Obshch. Khim.*, 1970, **40**, 57; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1970, **40**, 54 (*synth, uv*)

5-Iodotryptophan, 9CI, 8CI I-1-00066

2-Amino-3-(5-iodo-1H-indol-3-yl)propanoic acid



(*S*)-*form*

$C_{11}H_{11}IN_2O_2$ M 330.1

(S)-form [161295-03-0]
L-form
Off-white cryst. (70% EtOH). Mp 165-166°. $[\alpha]_D$ −12.3 (c, 1.08 in CF_3COOH).

(±)-form [15641-49-3]
Leaflets + $2H_2O$ (AcOH). Mp 264° (dihydrate).

Harvey, D.G., *J.C.S.*, 1958, 3760 (*synth*)
Ames, M.M. *et al*, *Synthesis*, 1994, 1433 (*S-form, synth, pmr*)

Isocyanoacetic acid, 9CI I-1-00067

[71804-44-9]

$CNCH_2COOH$

$C_3H_3NO_2$ M 85.0
Esters are reagents for cyclisation reactions.

Me ester: [39687-95-1].
$C_4H_5NO_2$ M 99.0 Liq. $Bp_{2.5}$ 77-79°.

Et ester: [2999-46-4].
$C_5H_7NO_2$ M 113.1 Liq. Bp_{11} 89-91°.

Benzyl ester: [41995-26-0].
$C_{10}H_9NO_2$ M 175.1 Pale brown solid. Mp 27.5-28.5°. $Bp_{0.075}$ 110-120°.

Amide: [51641-98-6].
$C_3H_4N_2O$ M 84.0 Cryst. Mp 122-123°.

Ugi, I. *et al*, *Angew. Chem.*, 1965, **77**, 492 (*Et ester*)
Damico, R. *et al*, *J.O.C.*, 1973, **38**, 3057 (*Me ester*)
Ozaki, Y. *et al*, *Synthesis*, 1979, 216 (*amide*)
Org. Synth., 1980, **59**, 183 (*Et ester*)
Lash, T.D. *et al*, *Synthesis*, 1994, 170 (*benzyl ester*)
Burns, D.H. *et al*, *Synth. Commun.*, 1995, **25**, 379 (*benzyl ester*)

Isocyanoacetonitrile I-1-00068

Cyanoisocyanomethane

$CNCH_2CN$

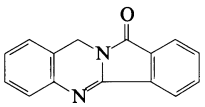
$C_3H_2N_2$ M 66.0
Cryst. solid at −30°. Mp −15°. Dec. rapidly > −10°.

Buschmann, J. *et al*, *Angew. Chem., Int. Ed.*, 1995, **34**, 914 (*synth, cmr, N-14 nmr*)

Isoindolo[1,2-*b*]quinazolin-12(10*H*)-one, 9CI I-1-00069

8-Desaminobatracylin

[35970-06-0]



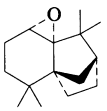
$C_{15}H_{10}N_2O$ M 234.2
Yellow needles (EtOH); cryst. (CH_2Cl_2/hexane). Mp 182-184°.

Gabriel, S., *Ber.*, 1912, **45**, 713 (*synth*)
Kametani, T. *et al*, *J. Het. Chem.*, 1971, **8**, 1071 (*synth, ir, pmr*)
Meegalla, S.K. *et al*, *J. Med. Chem.*, 1994, **37**, 3434 (*synth, ir, pmr, cmr*)

Isolongifolene epoxide I-1-00070

Octahydro-4,4,8,8-tetramethyl-4a,7-methano-4aH-naphth[1,8a-b]oxirene, 9CI. 8,8a-Epoxyoctahydro-1,1,5,5-tetramethyl-2H-2,4a-methanonaphthalene, 8CI. Folenox

[26619-69-2]

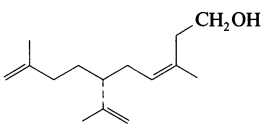


$C_{15}H_{24}O$ M 220.3
Struct. uncertain before 1974. Deodorising agent in perfumery. Cryst. (hexane). Mp 40-41.5°.

Eschinasi, E.H. *et al*, *Tet. Lett.*, 1970, 3523.
Ranganathan, R. *et al*, *Tetrahedron*, 1970, **26**, 621 (*synth, pmr, ir*)
McMillan, J.A. *et al*, *Tet. Lett.*, 1974, 419 (*cryst struct*)
Greengrass, C.W. *et al*, *Tetrahedron*, 1975, **31**, 689.

6-Isopropenyl-3,9-dimethyl-3,9-decadien-1-ol I-1-00071

3,9-Dimethyl-6-(1-methylethenyl)-3,9-decadien-1-ol, 9CI



(3*Z*,6*R*)-*form*

$C_{15}H_{26}O$ M 222.3

(3Z,6R)-form [73770-42-0]

Ac:
$C_{17}H_{28}O_2$ M 264.4 Sex pheromone of the female California red scale insect *Aonidiella aurantii.*

Propanoyl: [73416-54-3].
$C_{18}H_{30}O_2$ M 278.4 Sex pheromone of the female white peach scale, *Pseudoulacaspsis pentagona.* $[\alpha]_D^{25}$ +7.10 (c, 1.0 in $CHCl_3$) (≥99% op).

(3E,6R)-form [73770-43-1]
Propanoyl: [73770-44-2].
$[\alpha]_D^{25}$ +7.62 (c, 1.0 in $CHCl_3$).

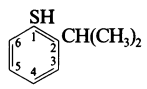
[73416-55-4, 127328-42-1]

Heath, R.R. *et al, J. Chem. Ecol.*, 1979, **5**, 941.
Heath, R.R. *et al, J.O.C.*, 1980, **45**, 2910 (*isol, synth, pmr, ir, ms*)
McLaughlin, J.R. *et al, J. Chem. Ecol.*, 1990, **16**, 749 (*activity*)
Kher, S.M. *et al, Synth. Commun.*, 1990, **20**, 495 (*synth, bibl, acetate*)

2-Isopropylbenzenethiol I-1-00072

2-(1-Methylethyl)benzenethiol, 9CI. o-*Cumenethiol, 8CI. 2-Isopropylthiophenol. 2-(2-Mercaptophenyl)propane*

[6262-87-9]



$C_9H_{12}S$ M 152.2
Liq. d 1.00. Bp 22°. n_D^{20} 1.5579.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1101A.
Hansch, C. *et al, J.A.C.S.*, 1948, **70**, 1561 (*synth*)
Atkinson, R.S. *et al, J.C.S. Perkin 2*, 1979, 1490 (*synth*)

4-Isopropylbenzenethiol I-1-00073

4-(1-Methylethyl)benzenethiol, 9CI. p-*Cumenethiol, 8CI. 4-Isopropylthiophenol. 2-(4-Mercaptophenyl)propane*

[4946-14-9]

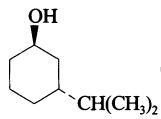
$C_9H_{12}S$ M 152.2
Liq. Bp_{14} 104-105°.

Gilman, H. *et al, J.A.C.S.*, 1947, **69**, 2053 (*synth*)
Schroth, W. *et al, Z. Chem.*, 1977, **17**, 411 (*synth*)

3-Isopropylcyclohexanol I-1-00074

3-(1-Methylethyl)cyclohexanol, 9CI

[4534-77-4]



(1*RS*,3*RS*)-*form*

$C_9H_{18}O$ M 142.2
Known in opt. active form as (1*S*- *cis*, *trans*-) mixt. (Van Osselaer *et al*).

(1RS,3RS)-form [64824-02-8]
(±)-trans-*form*
Viscous liq. d^{20} 0.92. Mp −6° to −5°. Bp_{15} 101°. n_D^{20} 1.4659.

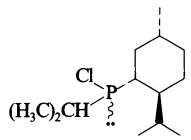
(1RS,3SR)-form [64824-01-7]
(±)-cis-*form*
Viscous liq. d^{20} 0.92. Mp −11° to −10°. Bp_{15} 106°. n_D^{20} 1.4651.

[69854-62-2, 69854-66-6, 87759-30-6, 87759-31-7]

Huckel, W. *et al, Chem. Ber.*, 1961, **94**, 96 (*synth*)
Van Osselaer, T.A. *et al, Bull. Soc. Chim. Belg.*, 1978, **87**, 799.
Merckx, E.M. *et al, Org. Magn. Reson.*, 1983, **21**, 380 (*pmr*)

Isopropyl(2-isopropyl-5-methylcyclohexyl) phosphinous chloride, 8CI I-1-00075

(1-Methylethyl)[5-methyl-2-(1-methylethyl) cyclohexyl]phosphinous chloride, 9CI



$C_{13}H_{26}ClP$ M 248.7

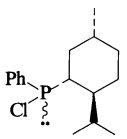
(1R,2S,5R)-form
Isopropylmenthylphosphinous chloride. Chloroisopropylmenthylphosphine
Liq. $Bp_{0.4}$ 112°. Diastereoisomers epimeric at P recognised spectroscopically.

[113613-08-4, 113629-75-7]

Hägele, G. *et al, J.C.S. Dalton*, 1987, 795 (*synth, pmr, cmr, P-31 nmr*)

(2-Isopropyl-5-methylcyclohexyl) phenylphosphinous chloride, 8CI I-1-00076

[*5-Methyl-2-(1-methylethyl)cyclohexyl*] *phenylphosphinous chloride, 9CI*



$C_{16}H_{24}ClP$ M 282.7

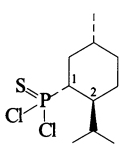
(1R,2S,5R)-form [103667-70-5]
Menthylphenylphosphinous chloride. Chloromenthylphenylphosphine
Liq. $Bp_{0.5}$ 135°. A mixt. of epimers at P (1:3) characterised spectroscopically.

[103667-69-2]

Boese, R. *et al, Chem.-Ztg.*, 1985, **109**, 233 (*synth, ms, cmr, P-31 nmr*)
Hägele, G. *et al, J.C.S. Dalton*, 1987, 795 (*synth, P-31 nmr, config*)

(2-Isopropyl-5-methylcyclohexyl) phosphonothioic dichloride I-1-00077

[*5-Methyl-2-(1-methylethyl)cyclohexyl*] *phosphonothioic dichloride*



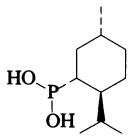
$C_{10}H_{19}Cl_2PS$ M 273.2

(1R,2S,5R)-form [103953-58-8]
Menthylphosphonothioic dichloride
Oil. $Bp_{0.3-0.4}$ 138-141°. Forms a cryst. adduct with 2-propanol.

Boese, R. *et al, Chem.-Ztg.*, 1985, **109**, 233 (*pmr, cmr*)
Hägele, G. *et al, Z. Naturforsch., B*, 1985, **40**, 1053 (*synth, pmr, cmr, P-31 nmr*)

(2-Isopropyl-5-methylcyclohexyl) phosphonous acid I-1-00078

[*5-Methyl-2-(1-methylethyl)cyclohexyl*] *phosphonous acid, 9CI*



$C_{10}H_{21}O_2P$ M 204.2

(1R,2S,5R)-form
(L-*Menthyl*)*phosphonous acid*

Di-Me ester: [83021-24-3]. *Dimethyl*(L-*menthyl*)*phosphonite*
$C_{12}H_{25}O_2P$ M 232.3 Liq. $Bp_{0.005}$ 49.5°. $[\alpha]_D^{15}$ −64.8 (c, 7.02 in C_6H_6).

Di-Et ester: [83021-25-4]. *Diethyl*(L-*menthyl*) *phosphonite*
$C_{14}H_{29}O_2P$ M 260.3 Liq. $Bp_{0.1}$ 83-87°. $[\alpha]_D^{15}$ −67.7 (c, 8.38 in C_6H_6).

Diisopropyl ester: [83021-26-5]. *Diisopropyl*(L-*menthyl*)*phosphonite*
$C_{16}H_{33}O_2P$ M 288.4 Liq. $Bp_{0.017}$ 68°. $[\alpha]_D^{15}$ −60.1 (c, 9.73 in C_6H_6).

Di-Ph ester: [83021-27-6]. *Diphenyl*(L-*menthyl*)*phosphonite*
$C_{22}H_{29}O_2P$ M 356.4 Liq. $Bp_{0.02}$ 153°. $[\alpha]_D^{15}$ −18.6 (c, 10.11 in C_6H_6).

Difluoride: (L-*Menthyl*)*phosphonous difluoride. Difluoro*(L-*menthyl*)*phosphine*
$C_{10}H_{19}F_2P$ M 208.2 No phys. props. reported.

Dichloride: [83021-21-0]. (L-*Menthyl*) *phosphonous dichloride. Dichloro*(L-*menthyl*)*phosphine*
$C_{10}H_{19}Cl_2P$ M 241.1 Pungent liq. $Bp_{0.1}$ 83-84°. $[\alpha]_D^{15}$ −113.6 (c, 8.24 in C_6H_6).

Diamide: see *3-(Diaminophosphinoyl)-p-menthane, D-1-00106*

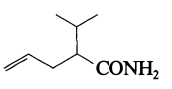
[93713-94-1, 93713-96-3]

Hidai, M. *et al, J. Organomet. Chem.*, 1982, **232**, 89 (*dichloride, esters, amide, synth, pmr*)
Feigel, M. *et al, Z. Naturforsch., B*, 1982, **37**, 1661 (*dichloride, pmr, cmr*)
Hinke, A. *et al, Phosphorus Sulfur Relat. Elem.*, 1983, **15**, 93 (*dichloride, synth, ms, pmr, P-31 nmr*)
Hägele, G. *et al, Z. Naturforsch., B*, 1985, **40**, 1053.
Graber, M. *et al, Phosphorus, Sulfur, Silicon Relat. Elem.*, 1989, **44**, 109 (*dichloride, synth, pmr, P-31 nmr*)

2-Isopropyl-4-pentenamide, 8CI I-1-00079

2-(1-Methylethyl)-4-pentenamide, 9CI. Allylisopropylacetamide

[299-78-5]



$C_8H_{15}NO$ M 141.2

Porphyrinogenic agent. Inducer of 5-aminolevulinic acid synthetase. Inhibits human epoxide hydrolase.

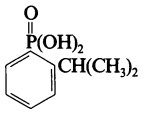
(±)-*form*
Mp 98-100°.

Freifelder, M. *et al*, *J.O.C.*, 1961, **26**, 203 (*synth*)
Granick, S., *J. Biol. Chem.*, 1963, **238**, PC2247 (*activity*)
Ortiz de Montellano, P.R. *et al*, *Arch. Biochem. Biophys.*, 1979, **197**, 524 (*bibl, activity*)
Prickett, K.S. *et al*, *Biomed. Mass Spectrom.*, 1984, **11**, 320 (*metab*)
Toshimitsu, A. *et al*, *J.O.C.*, 1987, **52**, 2018 (*synth, ir, pmr*)
Kerr, B.M. *et al*, *Drug Metab. Dispos.*, 1990, **18**, 540 (*metab*)

(2-Isopropylphenyl)phosphonic acid, 8CI I-1-00080

[2-(1-Methylethyl)phenyl]phosphonic acid, 9CI

[111192-82-6]



$C_9H_{13}O_3P$ M 200.1
Solid. Mp 173-174°. pK_{a1} 2.13; pK_{a2} 8.13 (H_2O, 25°).

[111193-12-5]

Nagarajan, K.N. *et al*, *Can. J. Chem.*, 1987, **65**, 1729 (*synth, props*)

(4-Isopropylphenyl)phosphonic acid, 8CI I-1-00081

[4-(1-Methylethyl)phenyl]phosphonic acid, 9CI

[128333-45-9]

$C_9H_{13}O_3P$ M 200.1

Di-Et ester: [51993-51-2]. *Diethyl (4-isopropylphenyl)phosphonate*
$C_{13}H_{21}O_3P$ M 256.2 Liq. Bp_1 140-142°.

Monohexyl ester: [128333-48-2]. *Monohexyl (4-isopropylphenyl)phosphonate*
$C_{15}H_{25}O_3P$ M 284.3 pK_a 3.53.

Dipropyl ester: Dipropyl [4-(1-methylethyl)phenyl]phosphonate
$C_{15}H_{25}O_3P$ M 284.3 Liq. d_4^{20} 1.02. Bp_4 156-157°.

Kharrasova, F.M. *et al*, *Zh. Obshch. Khim.*, 1973, **43**, 2642; *J. Gen. Chem. USSR (Engl. Transl.)*, 1973, **43**, 2621 (*ester, synth, P-31 nmr*)
Yuan, C. *et al*, *Synthesis*, 1990, 140 (*synth, P-31 nmr*)
Hu, W. *et al*, *Chin. Chem. Lett.*, 1992, **3**, 579 (*P-31 nmr*)
Yuan, C. *et al*, *Heteroat. Chem.*, 1993, **4**, 23 (*P-31 nmr*)

Isopropyl phenyl sulfide, 8CI I-1-00082

[(1-Methylethyl)thio]benzene, 9CI

[3019-20-3]

$PhSCH(CH_3)_2$

$C_9H_{12}S$ M 152.2
Liq. d^{20} 0.985. Bp 208°, Bp_{10} 87°. n_D^{20} 1.5464.

Adv. Chem. Ser., 1955, **15**, 179 (***props***)
Jones, I.W. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1978, **5**, 57 (*ms*)
Cogolli, P. *et al*, *J.O.C.*, 1979, **44**, 2642 (*synth, pmr*)

2-Isopropylthiophene, 8CI I-1-00083

2-(1-Methylethyl)thiophene, 9CI. 2-(2-Thienyl) propane

[4095-22-1]

$C_7H_{10}S$ M 126.2
Liq. d^{20} 0.968. Bp 154-155°, Bp_{14} 48-49°. n_D^{20} 1.5038.

Kutzi, W.M. *et al*, *J.A.C.S.*, 1946, **68**, 1977 (*synth*)
Adv. Chem. Ser., 1955, **15**, 194 (***props***)
Bedell, S.F. *et al*, *J.O.C.*, 1962, **27**, 2026 (*synth*)
Gouesnard, J.P. *et al*, *Bull. Soc. Chim. Fr.*, 1969, 4452 (*synth, pmr*)

3-Isopropylthiophene, 8CI I-1-00084

3-(1-Methylethyl)thiophene, 9CI. 2-(3-Thienyl) propane

[29488-27-5]

$C_7H_{10}S$ M 126.2
d^{20} 0.973. Bp 157°. n_D^{20} 1.5052.

Appleby, W.G. *et al*, *J.A.C.S.*, 1948, **70**, 1552 (*synth*)
Adv. Chem. Ser., 1955, **15**, 194 (***props***)
Pham, C.V. *et al*, *Synth. Commun.*, 1986, **16**, 689 (*synth, pmr*)

3-Isothiazolecarboxaldehyde I-1-00085

3-Formylisothiazole

[34490-97-6]

C_4H_3NOS M 113.1
Cryst. Mp 28-29°. Bp_9 62-65°. Unstable.

Oxime, (E-): [28401-56-1].
$C_4H_4N_2OS$ M 128.1 Cryst. (C_6H_6). Mp 76-77°.

2,4-Dinitrophenylhydrazone: Yellow needles (C_6H_6). Mp 225-227°.
Thiosemicarbazone: Prisms (EtOH). Mp 176-178° dec.

Jones, D.H. *et al*, *J.C.S.*, 1964, 3114 (*synth, uv*)
Benschop, H.P. *et al*, *J. Med. Chem.*, 1970, **13**, 1208 (*oxime*)

4-Isothiazolecarboxaldehyde I-1-00086

4-Formylisothiazole

[822-54-8]

C_4H_3NOS M 113.1
Cryst. (petrol). Mp 63° (58-60°).

Oxime, (E)-:
$C_4H_4N_2OS$ M 128.1 Cryst. (heptane/Et_2O). Mp 81-82°.

Oxime, (Z)-:
$C_4H_4N_2OS$ M 128.1 Cryst. (CCl_4). Mp 115-116°.

Ger. Pat., 1 179 553, (1964); *CA*, **62**, 565d (*synth*)
Benschop, H.P. *et al*, *J. Med. Chem.*, 1970, **13**, 1208 (*synth, oximes*)
Guilloteau, F. *et al*, *Synth. Commun.*, 1995, **25**, 1383 (*synth, ir, pmr, cmr*)

5-Isothiazolecarboxaldehyde I-1-00087

5-Formylisothiazole

[5242-57-9]

C_4H_3NOS M 113.1
Liq. Bp_{32} 95-98°.

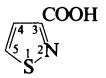
Oxime, (Z-): [28401-57-2].
$C_4H_4N_2OS$ M 128.1 Needles (C_6H_6). Mp 133-134°.

Phenylhydrazone: [73140-48-4].
Yellow prisms (EtOH). Mp 135-137°.
Thiosemicarbazone: Mp 192-194° dec.

Caton, M.P.L. *et al*, *J.C.S.*, 1964, 446 (*synth, uv*)
U.K. Pat., 1 012 620, (1965); *CA*, **64**, 5101g (*synth*)
Benschop, H.P. *et al*, *J. Med. Chem.*, 1970, **13**, 1208 (*synth, oxime*)
Faure, R. *et al*, *Can. J. Chem.*, 1975, **53**, 1677 (*cmr*)
Briggs, A.G. *et al*, *J.C.S. Perkin 1*, 1979, 2340 (*pmr, oxime*)

3-Isothiazolecarboxylic acid I-1-00088

[4576-90-3]



$C_4H_3NO_2S$ M 129.1
Needles (H_2O); cryst. (C_6H_6). Mp 137°.

Et ester: [23244-32-8].
$C_6H_7NO_2S$ M 157.1 Liq. Bp_5 140-145°.

Chloride: [49672-77-7].
C_4H_2ClNOS M 147.5 Mp 34-36°. Bp_{19} 123-124°.

Amide: [24342-43-6].
$C_4H_4N_2OS$ M 128.1 Needles (H_2O). Mp 154-155°.

Nitrile: [1452-17-1]. *3-Cyanoisothiazole*
$C_4H_2N_2S$ M 110.1 Prisms (petrol). Mp 60-61°.

Jones, D.H. *et al*, *J.C.S.*, 1964, 3114; 1965, 7277 (*synth, amide, nitrile, chloride, uv*)
Millard, B.J., *J.C.S.(C)*, 1969, 1231 (*ms*)
Noyce, D.S. *et al*, *J.O.C.*, 1975, **40**, 3381 (*Et ester*)

4-Isothiazolecarboxylic acid I-1-00089

[822-82-2]

$C_4H_3NO_2S$ M 129.1
Needles (H_2O). Mp 162-163°.

Me ester: [56133-37-0].
$C_5H_5NO_2S$ M 143.1 Needles (petrol). Mp 55°.

Et ester:
$C_6H_7NO_2S$ M 157.1 Yellow oil.

Chloride: [10271-90-6].
C_4H_2ClNOS M 147.5 Liq. $Bp_{2.5}$ 59.5-60°.

Amide: [24340-75-8].
$C_4H_4N_2OS$ M 128.1 Prisms (H_2O). Mp 192-193°.

Nitrile: [3912-37-6]. *4-Cyanoisothiazole*
$C_4H_2N_2S$ M 110.1 Cryst. Mp 95°. $Subl._{0.1}$ 50°.

Adams, A. *et al*, *J.C.S.*, 1959, 3061 (*synth, Me ester, amide*)
Raap, R. *et al*, *J. Med. Chem.*, 1968, **11**, 70 (*synth, nitrile, chloride*)
Benschop, H.P. *et al*, *J. Med. Chem.*, 1970, **13**, 1208 (*synth*)

Wasylishen, R.E. *et al*, *Can. J. Chem.*, 1975, **53**, 596 (*cmr*)
Apblett, A. *et al*, *Can. J. Chem.*, 1990, **68**, 650 (*nitrile*)
Guilloteau, F. *et al*, *Synth. Commun.*, 1995, **25**, 1383 (*Et ester*)

5-Isothiazolecarboxylic acid I-1-00090

[10271-85-9]

$C_4H_3NO_2S$ M 129.1
Cryst. (H_2O). Mp 201-202° dec.

Chloride: [3683-97-4].
C_4H_2ClNOS M 147.5 Liq. Bp_{26} 82°.

Amide: [3683-98-5].
$C_4H_4N_2OS$ M 128.1 Needles (H_2O). Mp 172-174°.

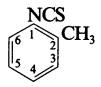
Nitrile: 5-Cyanoisothiazole
$C_4H_2N_2S$ M 110.1 Needles (petrol). Mp 47-48°.

Caton, M.P.L. *et al*, *J.C.S.*, 1964, 446 (*synth, uv*)
Caton, M.P.L. *et al*, *J. Med. Chem.*, 1965, **8**, 680 (*amide, nitrile, chloride*)
U.K. Pat., 1 012 620, (1965); *CA*, **64**, 5101g (*amide, nitrile, chloride*)

1-Isothiocyanato-2-methylbenzene, 9CI I-1-00091

o-*Tolyl isothiocyanate. 2-Methylphenyl isothiocyanate*

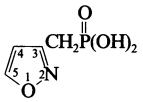
[614-69-7]



C_8H_7NS M 149.2
Yellow liq. d 1.11. Bp 239°, Bp_3 92-95°. n_D^{20} 1.64.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1423B.
Beilsteins Handbuch der Organischen Chemie, 4th edn., 12, 813.
Pak, C.S. *et al*, *Synthesis*, 1982, 969 (*synth*)
Furukawa, I. *et al*, *Chem. Express*, 1988, **3**, 215 (*synth*)
Prakash, L. *et al*, *J. Fluorine Chem.*, 1988, **41**, 303 (*synth*)
Dreikorn, B.A. *et al*, *J. Het. Chem.*, 1989, **26**, 1735 (*synth*)

(3-Isoxazolylmethyl) phosphonic acid I-1-00092



$C_4H_6NO_4P$ M 163.0

Di-Et ester: [97908-01-5]. *Diethyl (3-isoxazolylmethyl)phosphonate*
$C_8H_{14}NO_4P$ M 219.1 Liq.

Tsuge, O. *et al*, *Bull. Chem. Soc. Jpn.*, 1987, **60**, 2463 (*ester, synth, ir, ms, pmr, cmr*)

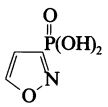
(5-Isoxazolylmethyl) phosphonic acid I-1-00093

$C_4H_6NO_4P$ M 163.0

Di-Et ester: [85167-83-5]. *Diethyl (5-isoxazolylmethyl)phosphonate*
$C_8H_{14}NO_4P$ M 219.1 Viscous liq. $Bp_{0.35}$ 110-115°.

De Shong, P. *et al*, *J.O.C.*, 1988, **53**, 1356 (*synth, ir, pmr, ms*)

3-Isoxazolylphosphonic acid I-1-00094



$C_3H_4NO_4P$ M 149.0

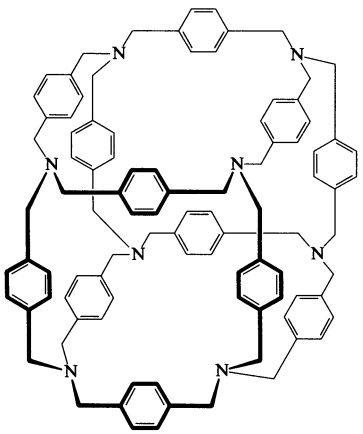
Di-Et ester: [130888-83-4]. *Diethyl 3-isoxazolylphosphonate*
$C_7H_{12}NO_4P$ M 205.1 Phys. props. not reported.

Zhang, R. *et al*, *Synthesis*, 1990, 817 (*synth, ir, pmr*)

K

Kyuphane **K-1-00001**

1,8,15,22,29,36,49,78-Octaazaheptadecacyclo
[27.13.13.13^{8,22}.6^{15,36}.6^{49,78}.2^{3,6}.2^{10,13}.2^{17,20}
.2^{24,27}.2^{31,34}.2^{38,41}.2^{44,47}.2^{51,54}.2^{63,66}.2^{73,76}
.2^{80,83}.2^{94,97}]tetrahecta-
3,5,10,12,17,19,24,26,31,33,38,40,44,46,51,
53,56,58,60,63,65,68,70,73,75,80,82,85,87,
89,91,94,96,99,101,103-hexatriacontaene, 9CI
[111457-62-6]



$C_{96}H_{96}N_8$ M 1361.8
Provides a hydrophobic binding site for anionic guest molecules. Solid. Mp 202° dec., Mp >373° dec.

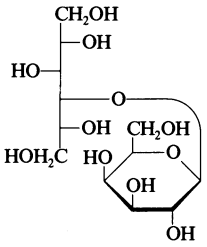
Murakami, Y. *et al*, *J.A.C.S.*, 1991, **113**, 8229 (*synth*, *pmr*, *cmr*, *ms*)
Takemura, H. *et al*, *J. Chem. Res., Synop.*, 1993, 424 (*synth*, *ms*, *pmr*)

L

Lactitol, BAN, INN **L-1-00001**

4-O-β-D-Galactopyranosyl-D-glucitol, 9CI. Emportal. Floralac. Importal. Oponaf. Portolac

[585-86-4]



$C_{12}H_{24}O_{11}$ M 344.3

Artificial sweetener used in foods. Monohydrate used in the management of hepatic encephalopathy. Also has laxative props. Cryst. + 1 or 2 H_2O.

▶ LD_{50} (rat, orl) 27500 mg/kg. LZ4392000.

[81025-03-8, 81025-04-9]

Hoagland, P.D. *et al, Carbohydr. Res.*, 1979, **74**, 135 (*cmr*)

Van Velthuijsen, J.A., *J. Agric. Food Chem.*, 1979, **27**, 680 (*rev, synth, props, use*); Kanters, J.A. *et al, Acta Cryst. C*, 1990, **46**, 2408 (*cryst struct*)

Van Velthuijsen, J.A. *et al, Food Sci. Technol.*, 1991, **48**, 283 (*rev*)

Kivikoski, J. *et al, Carbohydr. Res.*, 1992, **223**, 45, 53 (*cryst struct*)

Sinkledam, E.J. *et al, J. Am. Coll. Toxicol.*, 1992, **11**, 165, 189, 209, 219, 233, 249 (*tox*)

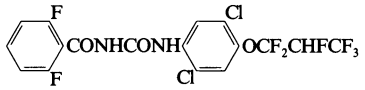
Christiansen-Brams, I. *et al, J. Carbohydr. Chem.*, 1992, **11**, 813 (*synth, pmr, cmr*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 1043.

Lufenuron, BAN, INN **L-1-00002**

N-[[[*2,5-Dichloro-4-(1,1,2,3,3,3-hexafluoropropoxy)phenyl]amino]carbonyl]-2,6-difluorobenzamide, 9CI. CGA 184699*

[103055-07-8]



$C_{17}H_8Cl_2F_8N_2O_3$ M 511.1

Insecticide. Chitin synth. inhibitor. Shows high activity against larvae of lepidopterous and coleopterous pests.

(+)-***form*** [130841-22-4]

Cryst. (toluene). Mp 166°. $[\alpha]_{368}^{24}$ +4 (c, 2 in $CHCl_3$).

(−)-***form*** [130841-26-8]

Mp 174-175°. $[\alpha]_{368}^{24}$ −3 (c, 2 in $CHCl_3$).

[103055-14-7, 110139-91-8]

Eur. Pat., 179 022, (1986) (*Ciba-Geigy*); *CA*, **105**, 37515j (*synth, activity*)

Ger. Pat., 4 000 335, (1990) (*Ciba-Geigy*); *CA*, **114**, 6041h (*synth, activity*)

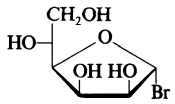
Buholzer, F. *et al, Meded. Fac. Landbouwwet., Rijksuniv. Gent*, 1992, **57**, 781 (*activity*)

MacKichan, J.J. *et al, J. Liq. Chromatogr.*, 1993, **16**, 2595 (*hplc*)

Wilson, E., *Chem. Eng. News*, July 31st, 1995, 16 (*rev*)

M

Mannofuranosyl bromide M-1-00001



α-D-*form*

$C_6H_{11}BrO_5$ M 243.0

α-D-form

Tetra-Ac: [55018-57-0].
$C_{14}H_{19}BrO_9$ M 411.2 Syrup.

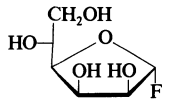
2,3:5,6-Di-O-isopropylidene: [38838-12-9].
$C_{12}H_{19}BrO_5$ M 323.1 Cryst. Mp 122-123°.

β-D-form

Tetra-Ac: [55018-58-1].
Syrup.

Hanessian, S. *et al, Carbohydr. Res.*, 1972, **24**, 45 (*diisopropylidene, pmr*)
Bock, K. *et al, Acta Chem. Scand., Ser. B*, 1974, **28**, 1041 (*tetra-Ac, pmr*)
McAdam, D.P. *et al, Aust. J. Chem.*, 1988, **41**, 563 (*tetra-Ac, diisopropylidene*)

Mannofuranosyl fluoride M-1-00002



α-D-*form*

$C_6H_{11}FO_5$ M 182.1

α-D-form

Tetra-Ac: [40031-25-2].
$C_{14}H_{19}FO_9$ M 350.2 Cryst. (Et_2O). Mp 96-97.5°. $[\alpha]_D^{25}$ +68.5 (c, 2.1 in $CHCl_3$).

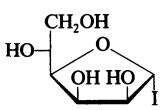
Tetrabenzoyl:
$C_{34}H_{27}FO_9$ M 598.5 Cryst. (Et_2O). Mp 90-91°. $[\alpha]_D^{23}$ −115.6 (c, 2 in $CHCl_3$).

β-D-form

Tetra-Ac: [40031-26-3].
Cryst. (Et_2O). Mp 91-92.5°. $[\alpha]_D^{25}$ −13.8 (c, 2.5 in $CHCl_3$).

Bock, K. *et al, Acta Chem. Scand.*, 1972, **26**, 2360 (*tetra-Ac, tetrabenzoyl, pmr, F-19 nmr*)
Bock, K. *et al, Acta Chem. Scand., Ser. B*, 1975, **29**, 682 (*cmr, F-19 nmr*)

Mannofuranosyl iodide M-1-00003



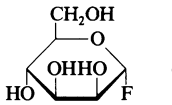
$C_6H_{11}IO_5$ M 290.0

α-D-form

2,3:5,6-Di-O-isopropylidene: [125181-25-1].
$C_{12}H_{19}IO_5$ M 370.1 Syrup.

Ernst, B. *et al, Tet. Lett.*, 1989, **30**, 3081 (*diisopropylidene, pmr*)

Mannopyranosyl fluoride M-1-00004



α-D-*form*

$C_6H_{11}FO_5$ M 182.1

α-D-form [2713-54-4]
Syrup.

Tetra-Ac: [2823-44-1].
$C_{14}H_{19}FO_9$ M 350.2 Cryst. (Et_2O/pentane). Mp 69-71°. $[\alpha]_D^{20}$ +22.7 (c, 2 in $CHCl_3$).

Tetrabenzoyl: [3825-18-1].
$C_{34}H_{27}FO_9$ M 598.5 Cryst. (Et_2O/pentane). Mp 129-131°. $[\alpha]_D^{20}$ −86.2 (c, 1.47 in $CHCl_3$).

4,6-Di-Me, 2-benzoyl: [69370-76-9].
$C_{15}H_{19}FO_6$ M 314.3 Cryst. (Et_2O/pentane). Mp 147-148°. $[\alpha]_D^{20}$ −36.3 (c, 1.5 in $CHCl_3$).

4,6-Di-Me, 2,3-dibenzoyl: [69370-75-8].
$C_{22}H_{23}FO_7$ M 418.4 Cryst. (pentane). Mp 79-81°. $[\alpha]_D^{20}$ −131.1 (c, 1.8 in $CHCl_3$).

β-D-form

Tetra-Ac: [57573-38-3].
Cryst. (Et_2O). Mp 105.5-107°. $[\alpha]_D^{20}$ −1 (c, 1.5 in $CHCl_3$).

4,6-Di-Me, 2-benzoyl: [69370-78-1].
Syrup.

4,6-Di-Me, 3-benzoyl: [69370-77-0].
$C_{15}H_{19}FO_6$ M 314.3 Syrup.

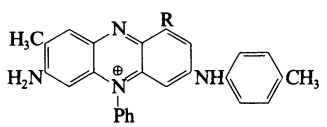
4,6-Di-Me, 2,3-dibenzoyl: [69370-79-2].
Syrup. $[\alpha]_D^{20}$ −82.2 (c, 2.5 in $CHCl_3$).

2,6-Anhydro: [108224-15-3].
$C_6H_9FO_4$ M 164.1 Solid. Mp 101-103.5°. $[\alpha]_D$ −66.8 (c, 1 in abs. EtOH).

Pedersen, C., *Acta Chem. Scand.*, 1963, **17**, 673 (*α-tetra-Ac, α-tetrabenzoyl*)
Hall, L.D. *et al, Can. J. Chem.*, 1969, **47**, 1 (*synth, pmr, F-19 nmr*)
Bock, K. *et al, Acta Chem. Scand., Ser. B*, 1975, **29**, 682 (*β-tetra-Ac, pmr, cmr*)
Pedersen, C. *et al, Acta Chem. Scand., Ser. B*, 1978, **32**, 687 (*Me deriv, pmr*)
Baillargeon, D.J. *et al, Carbohydr. Res.*, 1986, 154, 275 (*anhydro*)

Mauveine A M-1-00005

3-Amino-2-methyl-7-[(4-methylphenyl)amino]-5-phenylphenazinium



R = H

$C_{26}H_{23}N_4^{\oplus}$ M 391.4 (ion)
Derived by oxidn. of a mixt. of aniline and toluidines. Major component of Mauveine, a dye of historical importance. Purple solid (as chloride). The original struct. assigned to mauveine on little evidence was incorrect.
[153343-18-1]
Meth-Cohn, O. *et al, J.C.S. Perkin 1*, 1994, 5 (*struct, bibl*)

Mauveine B M-1-00006

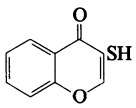
As Mauveine A, M-1-00005 with

R = CH_3

$C_{27}H_{25}N_4^{\oplus}$ M 405.5 (ion)
Derived by oxidn. of a mixt. of aniline and toluidines. Minor component of Mauveine. Purple solid (as chloride).
[153343-20-5]
Meth-Cohn, O. *et al, J.C.S. Perkin 1*, 1994, 5 (*struct, bibl*)

3-Mercapto-4*H*-1-benzopyran-4-one M-1-00007

3-Mercaptochromone



$C_9H_6O_2S$ M 178.2

S-*Me:* [39068-33-2]. *3-(Methylthio)-4H-1-benzopyran-4-one*
$C_{10}H_8O_2S$ M 192.2 Mp 111°.

S-*Et: 3-(Ethylthio)-4H-1-benzopyran-4-one*
$C_{11}H_{10}O_2S$ M 206.2 Mp 72°.

Yokoe, I. *et al, Chem. Pharm. Bull.*, 1994, **42**, 1697.

4-Mercapto-2-butanone M-1-00008

$HSCH_2CH_2COCH_3$

C_4H_8OS M 104.1

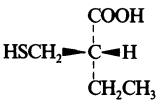
S-*Et: 4-(Ethylthio)-2-butanone*
$C_6H_{12}OS$ M 132.2 Oil. Bp_{17} 118-120°.

S-*Ph: 4-(Phenylthio)-2-butanone*
$C_{10}H_{12}OS$ M 180.2 Oil. Bp_{17} 173-175°.

Cain, M.E. *et al, J.C.S.*, 1962, 2959 (*derivs*)
Ozaki, Y. *et al, Chem. Pharm. Bull.*, 1995, **43**, 734 (*S-Et, S-Ph*)

2-(Mercaptomethyl)butanoic acid, 9CI M-1-00009

2-Ethyl-3-mercaptopropanoic acid
[133775-83-4]



(*S*)-*form*

$C_5H_{10}O_2S$ M 134.1

(*S*)-*form* [142569-51-5]
Oil which solidified on standing. Bp_2 102-104°. $[\alpha]_D$ −21.7 (c, 1.4 in $CHCl_3$).

(±)-*form* [147977-69-3]
Oil which solidified on standing. Bp_2 110-115°.

[147936-77-4]

Hutchinson, J.H. *et al*, *J. Het. Chem.*, 1994, **37**, 1153 (*synth, pmr*)

2-Mercapto-2-methylpropanal, 9CI M-1-00010

α-Mercaptoisobutanal

[89124-35-6]

$HSC(CH_3)_2CHO$

C_4H_8OS M 104.1
Liq. Bp 123°. Unstable, readily dimerises.

S-*Me:* [16042-21-0]. *2-Methyl-2-(methylthio) propanal*
$C_5H_{10}OS$ M 118.1 Liq. Bp 141°.

S-*Et:* [89812-32-8]. *2-(Ethylthio)-2-methylpropanal, 9CI*
$C_6H_{12}OS$ M 132.2 Oil.

Ethylene acetal: [135937-81-4]. *α,α-Dimethyl-1,3-dioxalane-2-methanethiol, 9CI*
$C_6H_{12}O_2S$ M 148.2 Oil.

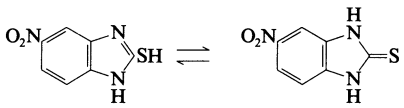
Disulfide: see *2,2'-Dithiobis[2-methylpropanal], D-1-00537*

Kirrmann, A. *et al*, *C. R. Hebd. Seances Acad. Sci.*, 1962, **255**, 728 (*S-Me, synth, ir, uv*)
Kirrmann, A. *et al*, *Bull. Soc. Chim. Fr.*, 1963, 1067 (*synth, uv, ir*)
McBride, B.J. *et al*, *J. Med. Chem.*, 1993, **36**, 81 (*deriv, synth, pmr*)

2-Mercapto-5-nitrobenzimidazole M-1-00011

1,3-Dihydro-5-nitro-2H-benzimidazole-2-thione, 9CI. 5-Nitro-1H-benzimidazole-2-thiol

[6325-91-3]



$C_7H_5N_3O_2S$ M 195.2
Exists in the thione form. Yellow cryst. (EtOH). Mp 280-281°.

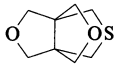
[2360-38-5]

Harrison, D. *et al*, *J.C.S.(B)*, 1967, 14 (*ir, tautom*)
Singh, S.P. *et al*, *J. Het. Chem.*, 1977, **14**, 1093 (*synth*)
Uchida, M. *et al*, *Chem. Pharm. Bull.*, 1989, **37**, 1517 (*synth*)

4H,6H-3a,6a-(Methanothiomethano)-1H,3H-furo[3,4-c]furan, 8CI M-1-00012

3,7-Dioxa-10-thia[3.3.3]propellane

[21533-86-8]

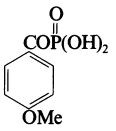


$C_8H_{12}O_2S$ M 172.2
Cryst. (MeOH). Mp 195-200°.

Altman, J. *et al*, *Tetrahedron*, 1969, **25**, 5115 (*synth, pmr*)

(4-Methoxybenzoyl) phosphonic acid M-1-00013

[66191-02-4]



$C_8H_9O_5P$ M 216.1

Monoanilinium salt: [67472-28-0]. Solid. Mp 183° dec.

Di-Me ester: [10570-48-6]. *Dimethyl (4-methoxybenzoyl)phosphonate*
$C_{10}H_{13}O_5P$ M 244.1 Liq. $Bp_{2.5}$ 170°.

Di-Me ester, 2,4-dinitrophenylhydrazone: Cryst. (MeOH). Mp 203-204°.

Di-Me ester, 4-methylbenzenesulfonylhydrazone: Solid. Mp 106° (stereoisomer. mixt.), Mp 138-140° (*anti* cryst. EtOH).

Di-Et ester: [16703-95-0]. *Diethyl (4-methoxybenzoyl)phosphonate*
$C_{12}H_{17}O_5P$ M 272.2 Liq. $Bp_{0.4}$ 158°.

Di-Et ester, 2,4-dinitrophenylhydrazone: Cryst. (MeOH). Mp 177-178°.

Diisopropyl ester: [41097-21-6]. *Diisopropyl (4-methoxybenzoyl)phosphonate*
$C_{14}H_{21}O_5P$ M 300.2 Liq. Dec. at bp.

Dibutyl ester: Dibutyl (4-methoxybenzoyl) phosphonate
$C_{16}H_{25}O_5P$ M 328.3 Liq. Bp_2 175°.

Dibutyl ester, 2,4-dinitrophenylhydrazone: Cryst. (MeOH). Mp 127-129°.

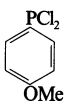
Bis(trimethylsilyl) ester: [66190-98-5]. *Bis(trimethylsilyl)(4-methoxybenzoyl) phosphonate*
$C_{14}H_{25}O_5PSi_2$ M 360.4 Liq. Bp_{10} 197-199°.

Berlin, K.D. *et al*, *J.A.C.S.*, 1964, **86**, 3862 (*synth, ir, pmr*)
Scherer, H. *et al*, *Chem. Ber.*, 1972, **105**, 3357 (*di-Me ester, deriv, ir, pmr*)
Clark, P.E. *et al*, *Phosphorus Relat. Group V Elem.*, 1973, **2**, 265 (*diisopropyl ester, ir, pmr, conformn*)
Sekine, M. *et al*, *Chem. Comm.*, 1978, 285 (*silyl ester, acid salt*)
Breuer, E. *et al*, *J.C.S. Perkin 1*, 1988, 3047 (*deriv, P-31 nmr*)
Krzyżanowska, B. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1988, **62**, 165 (*deriv, ms, ir, pmr, P-31 nmr*)
Dahn, H. *et al*, *Magn. Reson. Chem.*, 1990, **28**, 883 (*di-Me ester, O-17 nmr*)
Griffiths, D.V. *et al*, *J.C.S. Perkin 1*, 1992, 479 (*di-Me ester, synth, pmr, cmr, P-31 nmr*)

(4-Methoxyphenyl) phosphonous dichloride, 9CI M-1-00014

Dichloro(4-methoxyphenyl)phosphine

[19909-85-4]



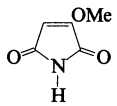
$C_7H_7Cl_2OP$ M 209.0
Ligand for Fe, Mn. Pungent, fairly unstable liq. Bp_{13} 150°, $Bp_{0.05}$ 74-78°.

Davies, W.C. *et al*, *J.C.S.*, 1944, 276 (*synth*)
Goetz, H. *et al*, *Annalen*, 1967, **704**, 1 (*synth*)
Miles, J.A. *et al*, *J.O.C.*, 1975, **40**, 343 (*synth, pmr*)
Zakirov, D.U. *et al*, *Zh. Obshch. Khim.*, 1977, **47**, 1661; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1977, **47**, 1522 (*nqr*)
Ratovskii, G.V. *et al*, *Zh. Obshch. Khim.*, 1992, **62**, 1797; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1992, **62**, 1477 (*uv, theory*)

3-Methoxy-1H-pyrrole-2,5-dione M-1-00015

Methoxymaleimide

[98027-61-3]



$C_5H_5NO_3$ M 127.0
Fine buff cryst. (diisopropyl ether). Mp 168.5-169°.

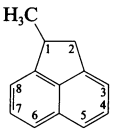
N-*Me:* [155071-29-7]. *3-Methoxy-1-methyl-1H-pyrrole-2,5-dione, 9CI*
$C_6H_7NO_3$ M 141.1 Soft yellow plates (hexane/C_6H_6). Mp 129-130°.

Rothhaas, A., *Annalen*, 1932, **501**, 295 (*synth*)
Gill, G.B. *et al*, *J.C.S. Perkin 1*, 1993, 2567 (*synth, ir, cmr*)

1-Methylacenaphthene M-1-00016

1,2-Dihydro-1-methylacenaphthylene, 9CI

[18086-45-8]



$C_{13}H_{12}$ M 168.2

(±)-form
$Bp_{1.2}$ 94°.

Bosch, A. *et al*, *Can. J. Chem.*, 1968, **46**, 715 (*synth, pmr*)
Bell, S.E.V. *et al*, *Aust. J. Chem.*, 1994, **47**, 1469 (*synth, pmr*)

3-Methylacenaphthene M-1-00017

1,2-Dihydro-3-methylacenaphthylene, 9CI

[39622-49-6]

$C_{13}H_{12}$ M 168.2
Cryst. (MeOH). Mp 58-60°.

Mitra, A. *et al*, *Indian J. Chem., Sect. B*, 1981, **20**, 449 (*synth*)
Kershaw, J.R., *Polycyclic Aromat. Compd.*, 1993, **3**, 185 (*ir, cmr, pmr, ms*)

4-Methylacenaphthene M-1-00018

1,2-Dihydro-4-methylacenaphthylene, 9CI, 8CI

[19345-96-1]

$C_{13}H_{12}$ M 168.2
Constit. of coal.

Kershaw, H.R., *Polycyclic Aromat. Compd.*, 1993, **3**, 185 (*ir, ms, pmr, cmr*)

5-Methylacenaphthene M-1-00019

1,2-Dihydro-5-methylacenaphthylene, 9CI, 8CI

[17057-80-6]

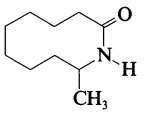
$C_{13}H_{12}$ M 168.2
Needles (EtOH). Mp 97°.

Cason, J. *et al*, *J.O.C.*, 1968, **33**, 3404 (*synth*)
Deady, L.W. *et al*, *J.O.C.*, 1972, **37**, 3335 (*synth*)

Kershaw, J.R., *Polycyclic Aromat. Compd.*, 1993, **3**, 185 (*ir, pmr, cmr, ms*)
Bell, S.E.V. *et al, Aust. J. Chem.*, 1994, **47**, 1469 (*synth, ir, pmr*)

10-Methylazacyclodecan-2-one M-1-00020

[134781-56-9]



$C_{10}H_{19}NO$ M 169.2

(±)-*form*
Solid. Mp 223-225°.

Bartra, M. *et al, J.O.C.*, 1991, **56**, 5132 (*synth, pmr, cmr, ir, ms*)

1-Methylazetidine, 9CI M-1-00021

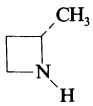
[4923-79-9]

C_4H_9N M 71.1
Liq. with ammoniacal odour. Bp_{735} 40°.
Picrate: Cryst. (C_6H_6). Mp 135-136°. Polymerises on standing.

Searles, S. *et al, J.A.C.S.*, 1956, **78**, 4917 (*synth*)
Maciel, G.E. *et al, J. Phys. Chem.*, 1965, **69**, 3925 (*cmr*)
Mazzocchi, P.H. *et al, J.O.C.*, 1979, **44**, 50 (*pmr, ir*)

2-Methylazetidine, 9CI M-1-00022

[19812-49-8]



(*S*)-*form*

C_4H_9N M 71.1

(*S*)-*form* [52265-79-9]
Liq. Bp 71-72°. $[\alpha]_D^{20}$ +11.6 (c, 1 in hexane). n_D^{20} 1.4208.

1-Me: [52265-80-2]. *1,2-Dimethylazetidine*
$C_5H_{11}N$ M 85.1 Liq. Bp 61°. $[\alpha]_D^{20}$ +43.5 (c, 1 in heptane).

(±)-*form* [52730-18-4]
Liq. with ammoniacal odour. Bp_{755} 72-76°.

Vaughan, W.R. *et al, J.O.C.*, 1961, **26**, 138 (*synth*)
Kostyanovsky, R.G. *et al, Org. Mass Spectrom.*, 1972, **6**, 661 (*ms*)
Kostyanovsky, R.G. *et al, Tetrahedron*, 1974, **30**, 39 (*resoln, uv, cd*)

3-Methylazetidine, 9CI M-1-00023

[35196-99-7]

C_4H_9N M 71.1
Liq. Bp 74-75°.

Higgins, R.H. *et al, J. Het. Chem.*, 1971, **8**, 531 (*synth, pmr*)

2-Methylbenzenemethanethiol, 9CI M-1-00024

2-Methylbenzyl mercaptan. 2-(Mercaptomethyl)toluene

[7341-24-4]

$C_8H_{10}S$ M 138.2
Liq. Bp_{14} 97°.

S-*Me:* [5925-79-1]. *1-Methyl-2[(methylthio) methyl]benzene, 9CI. Methyl 2-methylbenzyl sulfide*
$C_9H_{12}S$ M 152.2 Oil. Bp_{27} 122-123°.

Cagniant, P. *et al, Bull. Soc. Chim. Fr.*, 1961, 2225 (*synth*)
Oda, R. *et al, J.O.C.*, 1961, **26**, 4679 (*S-Me, synth*)
Padwa, A. *et al, Tetrahedron*, 1988, **44**, 4147 (*S-Me, synth*)

3-Methylbenzenemethanethiol, 9CI M-1-00025

3-Methylbenzyl mercaptan. 3-(Mercaptomethyl)toluene

[25697-56-7]

$C_8H_{10}S$ M 138.2
Liq. Bp_8 80-81°. n_D^{27} 1.5602.

Lombardino, J.G. *et al, J. Med. Chem.*, 1970, **13**, 206 (*synth*)

4-Methylbenzenemethanethiol, 9CI M-1-00026

4-Methylbenzyl mercaptan. 4-(Mercaptomethyl)toluene

[4498-99-1]

$C_8H_{10}S$ M 138.2
Liq. Bp_{30} 112-114°, Bp_{14} 99°.

S-*Me:* [5925-57-5]. *1-Methyl-4[(methylthio) methyl]benzene, 9CI. Methyl 4-methylbenzyl sulfide*
$C_9H_{12}S$ M 152.2 Oil. Bp_{30} 121°.

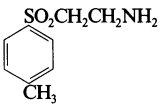
S-*Ph:* [5023-65-4]. *1-Methyl-4[(phenylthio) methyl]benzene, 9CI. 4-Methylbenzyl phenyl sulfide*
$C_{14}H_{14}S$ M 214.3 Cryst. (EtOH). Mp 69.0-70.1°.

Cagniant, P. *et al, Bull. Soc. Chim. Fr.*, 1961, 2225 (*synth*)
Molina, P. *et al, Synthesis*, 1982, 472 (*synth*)
Oae, S. *et al, Bull. Chem. Soc. Jpn.*, 1983, **56**, 248 (*S-Me, S-Ph*)
Olah, G.A. *et al, Synthesis*, 1994, 277 (*S-Me, synth*)

2-(4-Methylbenzenesulfonyl) ethylamine M-1-00027

2-[(4-Methylphenyl)sulfonyl]ethanamine, 9CI. β-Tosylethylamine

[50702-03-9]



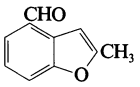
$C_9H_{13}NO_2S$ M 199.2
Reagent for *N*-protection of amides, carbamates and related compds. Cryst. (C_6H_6/petrol). Mp 66-67° (62.5-64°).

Madinaveitia, J. *et al, Biochem. J.*, 1945, **39**, 85 (*synth*)
Di Pietro, D. *et al, J.O.C.*, 1994, **59**, 5856 (*synth, use, pmr*)

2-Methyl-4-benzofurancarboxaldehyde, 9CI M-1-00028

Habropetalal

[71641-09-3]



$C_{10}H_8O_2$ M 160.1
Isol. from the fish-stunning plant *Habropetalum dawei*. Pale yellow oil. $Bp_{0.1}$ 80°.

Hanson, S.W. *et al, Phytochemistry*, 1981, **20**, 1162 (*isol*)

3-Methyl-2-benzofurancarboxaldehyde, 9CI M-1-00029

[1199-07-1]

$C_{10}H_8O_2$ M 160.1
Cryst. (MeOH or petrol). Mp 65°.

Bisagni, E. *et al, Bull. Soc. Chim. Fr.*, 1962, 925 (*synth*)
Deorna, D.S. *et al, Chem. Ber.*, 1964, **98**, 3577 (*synth*)
Saari, W.S. *et al, J. Med. Chem.*, 1992, **35**, 3792 (*synth, pmr*)

4-Methyl-2-benzofurancarboxaldehyde, 9CI M-1-00030

[53715-91-6]

$C_{10}H_8O_2$ M 160.1
Needles (cyclohexane/petrol). Mp 57.5°. Bp_9 141°.

Platzer, N. *et al, Bull. Soc. Chim. Fr.*, 1974, 905 (*synth*)

4-Methyl-5-benzofurancarboxaldehyde, 9CI M-1-00031

[119795-37-8]

$C_{10}H_8O_2$ M 160.1
Pale peach solid. Mp 66-67°.

Hammond, M.L. *et al, J. Med. Chem.*, 1989, **32**, 1006 (*synth, pmr*)

5-Methyl-2-benzofurancarboxaldehyde, 9CI M-1-00032

[40724-03-6]

$C_{10}H_8O_2$ M 160.1
Microcryst. (petrol). Mp 28.5°. Bp_{10} 143°.

Platzer, N. *et al, Bull. Soc. Chim. Fr.*, 1974, 905 (*synth*)

5-Methyl-3-benzofurancarboxaldehyde, 9CI M-1-00033

[143883-36-7]

$C_{10}H_8O_2$ M 160.1

Liq.

Deshpande, A.R. *et al*, *Indian J. Chem., Sect. B*, 1992, **31**, 526 (*synth, ir, pmr*)

6-Methyl-2-benzofurancarboxaldehyde, 9CI M-1-00034

[53715-92-7]

$C_{10}H_8O_2$ M 160.1
Prisms (petrol). Mp 36°. Bp_{10} 146°.

Platzer, N. *et al*, *Bull. Soc. Chim. Fr.*, 1974, 905 (*synth*)

6-Methyl-3-benzofurancarboxaldehyde, 9CI M-1-00035

[143883-37-8]

$C_{10}H_8O_2$ M 160.1
Liq.

Deshpande, A.R. *et al*, *Indian J. Chem., Sect. B*, 1992, **31**, 526 (*synth, ir, pmr*)

7-Methyl-2-benzofurancarboxaldehyde, 9CI M-1-00036

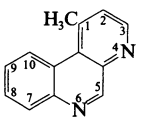
[57897-70-8]

$C_{10}H_8O_2$ M 160.1
Flavour enhancer for coffee.

U.S. Pat., 4 002 793, (1977) (*Firmenich*); *CA*, **86**, 171246p (*synth, use*)

1-Methylbenzo[*f*][1,7]naphthyridine, 9CI M-1-00037

[155050-59-2]

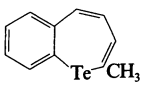


$C_{13}H_{10}N_2$ M 194.2
Cryst. (heptane). Mp 89-90°.

Chrzastek, L. *et al*, *Aust. J. Chem.*, 1994, **47**, 2129 (*synth, pmr*)

2-Methyl-1-benzotellurepin, 9CI M-1-00038

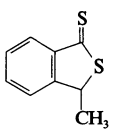
[153140-88-6]



$C_{11}H_{10}Te$ M 269.8
Viscous orange-red oil. Unstable, gradually dec. Higher homologues also prepd.

Sashida, H. *et al*, *Chem. Pharm. Bull.*, 1995, **43**, 19 (*synth, pmr*)

3-Methylbenzo[*c*]thiophene-1(3*H*)-thione M-1-00039



$C_9H_8S_2$ M 180.2

(±)-*form*
Liq. Bp_3 155°.

Nishio, T., *J.C.S. Perkin 1*, 1995, 561 (*synth, ir, pmr, cmr*)

3-Methyl-2-buten-1-amine, 9CI M-1-00040

3-Methyl-2-butenylamine, 8CI. 3,3-Dimethylallylamine. 1-Amino-3-methyl-2-butene. Prenylamine†

[13822-06-5]

$(H_3C)_2C{=}CHCH_2NH_2$

$C_5H_{11}N$ M 85.1
Oil. d_4^{20} 0.8010. Bp 109.5-111°. n_D^{20} 1.4423.
Hydrochloride: [26728-58-5].
Cryst. (EtOH). Mp 201°.
Picrate: Cryst. (EtOAc/C_6H_6). Mp 138.6-139.2°.
Ac: [73286-69-8].
$C_7H_{13}NO$ M 127.1 Oil.

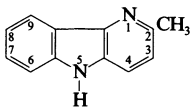
[108963-90-2]

Semenow, D. *et al*, *J.A.C.S.*, 1958, **80**, 5472 (*synth*)
Desvages, G. *et al*, *Bull. Soc. Chim. Fr.*, 1969, 3229; 1970, 1938 (*synth*)
Stotskii, A.A. *et al*, *Zh. Org. Khim.*, 1971, **7**, 2081; 1976, **12**, 1650; *J. Org. Chem. USSR* (*Engl. Transl.*), 1971, **7**, 2162; 1976, **12**, 1625 (*synth, ir, pmr*)
Montgomery, J.A. *et al*, *J. Med. Chem.*, 1977, **20**, 116 (*synth, pmr, cmr*)
Deslongchamps, P. *et al*, *Chem. Heterocycl. Compd.*, 1979, **57**, 3262 (*synth, pmr*)
Chen, S.C. *et al*, *Agric. Biol. Chem.*, 1982, **46**, 2361 (*cmr*)
Murahashi, S. *et al*, *J.O.C.*, 1989, **54**, 3292 (*synth, pmr*)
Crombie, L. *et al*, *J.C.S. Perkin 1*, 1992, 3179 (*synth, pmr*)
Ramalingam, K. *et al*, *Synth. Commun.*, 1995, **25**, 743 (*synth, acetate*)

2-Methyl-δ-carboline M-1-00041

*2-Methyl-5*H*-pyrido[3,2-b]indole, 9CI*

[78121-16-1]



$C_{12}H_{10}N_2$ M 182.2
Cryst. (C_6H_6/petrol). Mp 275°.

Sevodin, V.P. *et al*, *Khim. Geterotsikl. Soedin.*, 1981, 368; *Chem. Heterocycl. Compd.* (*Engl. Transl.*), 1981, 271 (*synth, uv, pmr*)

4-Methyl-δ-carboline M-1-00042

*4-Methyl-5*H*-pyrido[3,2-b]indole, 9CI*

[78121-17-2]

$C_{12}H_{10}N_2$ M 182.2
Cryst. (C_6H_6/petrol). Mp 264-265°.

Sevodin, V.P. *et al*, *Khim. Geterotsikl. Soedin.*, 1981, 368; *Chem. Heterocycl. Compd.* (*Engl. Transl.*), 1981, 271 (*synth, uv, pmr*)
Quéguiner, G. *et al*, *J.O.C.*, 1993, **58**, 7832 (*synth, pmr, cmr, ir*)

Methylcyanamide, 9CI M-1-00043

Methylcarbodiimide

[4674-68-4]

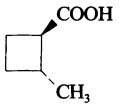
MeNHCN

$C_2H_4N_2$ M 56.0
Liq. Mp −40° to −50°. Nondistillable. Polym. on standing to give trimethylmelamine (see under 1,3,5-Triazine-2,4,6-triamine, T-0-03623). Can be stored as cryst. at −78°.

Baum, F. *et al*, *Ber.*, 1908, **41**, 524 (*synth*)
Kitawaki, R. *et al*, *J.O.C.*, 1960, **25**, 1043 (*synth*)
Cockerill, A.F. *et al*, *Synthesis*, 1976, 591 (*synth*)

2-Methylcyclobutanecarboxylic acid M-1-00044

[42185-61-5]



(1*RS*,2*RS*)-*form*

$C_6H_{10}O_2$ M 114.1
In later lit. *cis* and *trans* isomers were sep. by glc and characterised by pmr. *trans*-Isomer descr. below may be a mixt. of isomers.

***(1RS,2RS)*-form** [57705-61-0]
(±)-trans-*form*
Liq. with unpleasant cheese-like odour. Bp 200°.

Et ester:
$C_8H_{14}O_2$ M 142.1 d_{25}^{25} 0.94. Bp 161-164°.

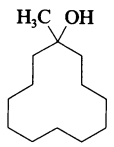
Amide:
$C_6H_{11}NO$ M 113.1 Cryst. (C_6H_6/pentane). Mp 130-131.5°.

[57705-60-9]

Blomquist, A.T. *et al*, *J.O.C.*, 1956, **21**, 1371 (*synth*)
Silver, M.S. *et al*, *J.A.C.S.*, 1961, **83**, 3671 (*synth*)
Gol'mov, V.P. *et al*, *Zh. Org. Khim.*, 1966, **2**, 2159; *J. Org. Chem. USSR* (*Engl. Transl.*), 1966, **2**, 2116 (*synth*)
Hill, E.A. *et al*, *J.A.C.S.*, 1976, **98**, 167 (*synth, pmr, bibl*)
Török, B. *et al*, *J.C.S. Perkin 1*, 1993, 801 (*synth, ms, pmr*)

1-Methyl-1-cyclododecanol M-1-00045

[32400-09-2]



$C_{13}H_{26}O$ M 198.3
Cryst. (petrol). Mp 91-92.5°.

Me ether: [37514-30-0]. *1-Methoxy-1-methylcyclododecane. Madrox*
$C_{14}H_{28}O$ M 212.3 Used in perfumery.
Liq. d 0.92.

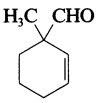
[26600-63-5]

Sicher, J. *et al*, *Coll. Czech. Chem. Comm.*, 1971, **36**, 3633; *CA*, **76**, 85240v (*synth*)
Ger. Pat., 2 152 016, (1972); *CA*, **77**, 47952s.
Swiss Pat., 550 344, (1974); *CA*, **82**, 47636v.
Ger. Pat., 2 852 344, (1980); *CA*, **93**, 220427e.
Archer, M. *et al*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1982, **79**, 227 (*cmr*)

1-Methyl-2-cyclohexene-1-carboxaldehyde, 9CI M-1-00046

3-Formyl-3-methylcyclohexene

[22911-31-5]



$C_8H_{12}O$ M 124.1

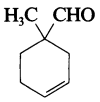
(±)-***form*** [66088-40-2]
Liq. Bp_{12} 60-70°.

Nerdel, F. *et al*, *Chem. Ber.*, 1969, **102**, 407 (*synth, ir, pmr*)

1-Methyl-3-cyclohexene-1-carboxaldehyde, 9CI M-1-00047

4-Formyl-4-methylcyclohexene

[931-96-4]



$C_8H_{12}O$ M 124.1

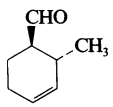
(±)-***form*** [112622-02-3]
Bp 164-166°, Bp_{27} 74°. n_D^{20} 1.4640.

Semicarbazone: Cryst. Mp 174°.

Pines, H. *et al*, *J.A.C.S.*, 1951, **73**, 5738 (*synth*)
Berkowitz, W.F. *et al*, *J.O.C.*, 1976, **41**, 10 (*synth, ir, pmr*)

2-Methyl-3-cyclohexene-1-carboxaldehyde, 9CI M-1-00048

[17775-58-5]



(1*RS*,2*RS*)-*form*

$C_8H_{12}O$ M 124.1

(***1RS,2RS***)-***form*** [766-48-3]
(±)-trans-*form*
Liq. Bp_{15} 56-57°.

Semicarbazone: Mp 141-143° (139-140°).

(***1RS,2SR***)-***form*** [873-30-3]
(±)-cis-*form*
Liq. Bp_{12} 60-61°. n_D^{20} 1.4732 (1.4780).

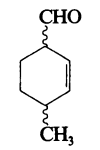
Semicarbazone: [709-37-5].
Mp 196-197° (181.5-183°).

Alder, K. *et al*, *Annalen*, 1949, **564**, 120 (*synth*)
Büchi, G. *et al*, *J.A.C.S.*, 1970, **92**, 3126 (*synth, pmr*)
Kugatova-Shemyakina, G.P. *et al*, *Zh. Org. Khim.*, 1970, **6**, 2446; *J. Org. Chem. USSR (Engl. Transl.)*, 1970, **6**, 2459 (*synth*)

4-Methyl-2-cyclohexene-1-carboxaldehyde, 9CI M-1-00049

3-Formyl-6-methylcyclohexene

[19876-38-1]



$C_8H_{12}O$ M 124.1

Liq. Bp_6 55-60°. n_D^{20} 1.487.

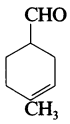
Semicarbazone: [19876-39-2].
Cryst. (EtOH aq.). Mp 136-137°.

Vig, O.P. *et al*, *Indian J. Chem.*, 1967, **5**, 541 (*synth, ir*)

4-Methyl-3-cyclohexene-1-carboxaldehyde, 9CI M-1-00050

4-Formyl-1-methylcyclohexene

[7560-64-7]



$C_8H_{12}O$ M 124.1

(±)-***form*** [61426-17-3]
Liq. Bp_{22} 79-80°. n_D^{20} 1.4708.

Semicarbazone: [27312-86-3].
Plates (EtOH). Mp 162-163.5°.

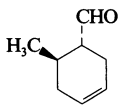
Di-Me acetal: [66334-23-4]. *4-(Dimethoxymethyl)-1-methylcyclohexene, 9CI*
$C_{10}H_{18}O_2$ M 170.2 Liq. $Bp_{0.25}$ 63°.

Di-Et acetal: [80825-36-1]. *4-(Diethoxymethyl)-1-methylcyclohexene, 9CI*
$C_{12}H_{22}O_2$ M 198.3 Liq. Bp_{12} 105-107°.

Kugatova, G. *et al*, *Zh. Obshch. Khim.*, 1957, **27**, 2450; 1960, **30**, 3731; *J. Gen. Chem. USSR (Engl. Transl.)*, 1957, **27**, 2511; 1960, **30**, 3696 (*synth*)
Büchi, G. *et al*, *J.A.C.S.*, 1970, **92**, 3126 (*synth*)
Nakagawa, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1977, **50**, 2487 (*cmr*)
Dolby, L. *et al*, *J.O.C.*, 1977, **42**, 1607 (*synth, ir, pmr*)
Ipaktschi, J., *Z. Naturforsch., B*, 1986, **41**, 496 (*synth, pmr*)
Carpita, A. *et al*, *Synth. Commun.*, 1994, **24**, 3167 (*synth*)

6-Methyl-3-cyclohexene-1-carboxaldehyde, 9CI M-1-00051

[89-94-1]



(1*RS*,6*RS*)-*form*

$C_8H_{12}O$ M 124.1

(***1RS,6RS***)-***form*** [36635-33-3]
(±)-trans-*form*
Liq. Bp_{13} 63°. n_D^{20} 1.4680.

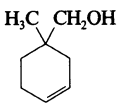
Semicarbazone: [39163-61-6].
Mp 169°.

Diels, O. *et al*, *Annalen*, 1929, **470**, 62 (*synth*)
Alder, K. *et al*, *Annalen*, 1949, **564**, 120 (*synth*)
Bazyl'chik, V.V. *et al*, *Zh. Org. Khim.*, 1985, **21**, 1450 (*synth*)

1-Methyl-3-cyclohexene-1-methanol, 9CI M-1-00052

4-Hydroxymethyl-4-methylcyclohexene

[50552-10-8]



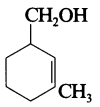
$C_8H_{14}O$ M 126.1

(±)-***form***
Liq. Bp_{35} 116°. n_D^{26} 1.4859.

Nouguier, R. *et al*, *Bull. Soc. Chim. Fr.*, 1973, 2399 (*synth*)

3-Methyl-2-cyclohexene-1-methanol, 9CI M-1-00053

3-Hydroxymethyl-1-methylcyclohexene



$C_8H_{14}O$ M 126.1

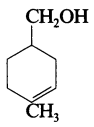
(±)-***form*** [98442-48-9]
Liq. Bp_1 55-63°.

Inouye, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 3492 (*synth, ir, pmr*)

4-Methyl-3-cyclohexene-1-methanol, 9CI M-1-00054

4-Hydroxymethyl-1-methylcyclohexene

[39155-38-9]



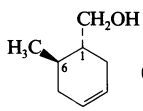
$C_8H_{14}O$ M 126.1

(±)-***form*** [89690-46-0]
Liq. Bp_{20} 108-109°, Bp_9 92°. n_D^{26} 1.4575.

Nouguier, R. *et al*, *Bull. Soc. Chim. Fr.*, 1973, 2399 (*synth*)
Monti, S.A. *et al*, *J.O.C.*, 1975, **40**, 215 (*synth, pmr*)
Carpita, A. *et al*, *Synth. Commun.*, 1994, **24**, 3167 (*synth*)

6-Methyl-3-cyclohexene-1-methanol, 9CI M-1-00055

4-Hydroxymethyl-5-methylcyclohexene



(1*R*,6*R*)-*form*

$C_8H_{14}O$ M 126.1

(***1R,6R***)-***form*** [92344-77-9]
(−)-trans-*form*
Liq. Bp_{21} 100-109°. $[\alpha]_D^{23}$ −75.4 (c, 6.63 in $CHCl_3$).

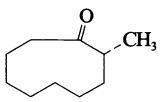
(***1R,6S***)-***form*** [102629-34-5]
Liq. Bp_{37} 120-122°. $[\alpha]_D^{26}$ −25.58 (c, 0.995 in $CHCl_3$).

(***1S,6S***)-***form*** [92344-78-0]
(+)-cis-*form*
Liq. Bp_{21} 100-109°. $[\alpha]_D^{23}$ +70.6 (c, 6.82 in $CHCl_3$).

Sonnet, P.E. *et al*, *J.O.C.*, 1984, **49**, 4639 (*1R6R-form, synth, pmr*)
Clive, D.L.J. *et al*, *J.O.C.*, 1986, **51**, 2717 (*1R6S-form, synth, pmr*)
U.S. Pat., 5 072 002, (1991); *CA*, **116**, 173892j (*1R6S-form, synth, pmr*)

2-Methylcyclononanone, 9CI M-1-00056

[73674-37-0]



(*R*)-*form*

$C_{10}H_{18}O$ M 154.2

(R)-form

Oil. $[\alpha]_D^{23}$ −19.3 (c, 0.23 in $CHCl_3$).

(±)-form [141884-17-5]

Oil. Bp_{15} 108°.

2,4-Dinitrophenylhydrazone: [73674-40-5]. Mp 123-124°.

Semicarbazone: Mp 144-145°.

Müller, E. *et al*, *Annalen*, 1962, **654**, 92 (*synth*)
Suzuki, S. *et al*, *Agric. Biol. Chem.*, 1987, **51**, 3095 (*synth, pmr*)
Baldwin, J.E. *et al*, *Tetrahedron*, 1992, **48**, 3385 (*synth, ir, pmr*)
Satoh, T. *et al*, *Tetrahedron*, 1994, **50**, 11839 (*synth, ir, pmr, ms*)
Enders, D. *et al*, *Annalen*, 1995, 1127 (*R-form, synth, ir, pmr, cmr, ms*)

5-Methylcyclononanone, 9CI M-1-00057

[80926-31-4]

$C_{10}H_{18}O$ M 154.2

(±)-form

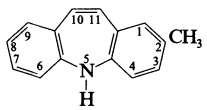
Liq. Bp_{10} 99°. n_D^{25} 1.4714.

Semicarbazone: Mp 167-168°.

Blomquist, A.T. *et al*, *J.A.C.S.*, 1958, **80**, 630 (*synth*)

2-Methyl-5*H*-dibenz[*b,f*]azepine M-1-00058

[70401-31-9]



$C_{15}H_{13}N$ M 207.2

Yellow plates (EtOH). Mp 164-166°.

Patton, J.R. *et al*, *J. Het. Chem.*, 1979, **16**, 257 (*synth, uv, ir*)
Tokmakov, G.P. *et al*, *Tetrahedron*, 1995, **51**, 2091 (*synth, uv, pmr, ms*)

3-Methyl-5*H*-dibenz[*b,f*]azepine M-1-00059

$C_{15}H_{13}N$ M 207.2

Yellow plates (C_6H_6). Mp 213-215°.

Tokmakov, G.P. *et al*, *Tetrahedron*, 1995, **51**, 2091 (*synth, uv, pmr*)

4-Methyl-5*H*-dibenz[*b,f*]azepine M-1-00060

$C_{15}H_{13}N$ M 207.2

Orange cryst. (hexane). Mp 85-87°.

Tokmakov, G.P. *et al*, *Tetrahedron*, 1995, **51**, 2091 (*synth, uv, pmr*)

10-Methyl-5*H*-dibenz[*b,f*]azepine M-1-00061

[92552-17-5]

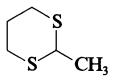
$C_{15}H_{13}N$ M 207.2

Light yellow cryst. (hexane). Mp 133-134°.

Ger. Pat., 1 142 870, (1963); *CA*, **59**, 11454e.
Groth, U. *et al*, *Annalen*, 1992, 199 (*synth, ir, pmr, cmr*)
Tokmakov, G.P. *et al*, *Tetrahedron*, 1995, **51**, 2091 (*synth, uv, pmr, ms*)

2-Methyl-1,3-dithiane M-1-00062

[6007-26-7]



$C_5H_{10}S_2$ M 134.2

Liq. d 1.12. Bp_3 56-59°. n_D^{20} 1.5610.

1-Oxide, (cis-)*:* [60349-78-2].
$C_5H_{10}OS_2$ M 150.2 Cryst. (Et_2O). Mp 60-62°.

1-Oxide, (trans-)*:* [60349-75-9].
Cryst. (CH_2Cl_2/Et_2O). Mp 92-94°.

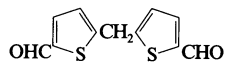
[16452-25-8, 87480-75-9, 87480-78-2, 87480-80-6, 87480-81-7, 99211-34-4, 99211-37-7, 134168-36-8]

Carey, F.A. *et al*, *J.O.C.*, 1976, **41**, 3975; 1978, **43**, 96 (*synth, ir, pmr, cmr, oxides*)
Rodriguez, A.D. *et al*, *Tetrahedron*, 1985, **41**, 4443 (*synth, pmr*)
Soderquist, J.A. *et al*, *Tet. Lett.*, 1986, **27**, 6305 (*synth*)
Page, P.C.B. *et al*, *Synlett*, 1991, 80 (*oxides*)
Barkley, J. *et al*, *Acta Cryst. C*, 1992, **48**, 2039 (*cryst struct, trioxide*)

5,5′-Methylenebis-2-thiophenecarboxaldehyde, 9CI M-1-00063

5,5′-Diformyl-2,2′-dithienylmethane

[32928-33-9]



$C_{11}H_8O_2S_2$ M 236.3

Prisms (petrol). Mp 95°.

Ahmed, M. *et al*, *J.C.S.(C)*, 1971, 2104 (*synth, ir, pmr*)
Hu, Z. *et al*, *J.O.C.*, 1994, **59**, 8071 (*synth, pmr, cmr, ms*)

3-Methylenecyclohexanol M-1-00064

[6749-63-9]

$C_7H_{12}O$ M 112.1

(±)-form [97551-97-8]

Bp 172-174°. n_D^{25} 1.4797.

[22445-56-3, 97551-97-8]

Albisetti, C.J. *et al*, *J.A.C.S.*, 1956, **78**, 2637 (*synth*)
Lambert, J.B. *et al*, *J.A.C.S.*, 1976, **98**, 4203 (*conformn*)
Brown, J.M. *et al*, *Tet. Lett.*, 1984, **25**, 1393 (*synth*)

4-Methylenecyclohexanol, 9CI M-1-00065

[22428-85-9]

$C_7H_{12}O$ M 112.1

Bp_{16} 78°.

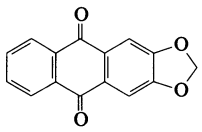
4-Methylbenzenesulfonyl: [89029-65-2]. Cryst.

Stolow, R.D. *et al*, *Tet. Lett.*, 1968, 5781 (*conformn, pmr*)
Bocelli, G. *et al*, *J. Mol. Struct.*, 1983, **102**, 39 (*cryst struct, deriv*)
Ishiyama, J. *et al*, *Bull. Chem. Soc. Jpn.*, 1987, **60**, 1721 (*synth, ir, cmr*)
Kirmse, W. *et al*, *Chem. Ber.*, 1987, **120**, 839 (*synth*)

2,3-Methylenedioxyanthraquinone M-1-00066

*Anthra[2,3-*d*]-1,3-dioxole-5,10-dione, 9CI*

[107996-98-5]



$C_{15}H_8O_4$ M 252.2

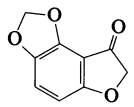
Yellow needles (EtOAc). Mp 225-226°.

Khanapure, S.P. *et al*, *J. Nat. Prod.*, 1989, **52**, 1357 (*synth, ir, pmr, cmr, ms*)

6,7-Methylenedioxyphthalide M-1-00067

*Furo[3,4-*e*]-1,3-benzodioxol-8(6*H*)-one, 9CI.*
*6,7-Methylenedioxy-1(3*H*)-isobenzofuranone.*
Coryhumolide

[4741-65-5]



$C_9H_6O_4$ M 178.1

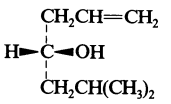
Isol. from tuber tissue of *Corydalis humosa*. Mp 236-238° (230-232°).

Hughes, D.W. *et al*, *Can. J. Chem.*, 1976, **54**, 2252 (*cmr*)
Cushman, M. *et al*, *J.O.C.*, 1980, **45**, 5067 (*synth, ir, pmr, ms*)
Hung, T.V. *et al*, *Aust. J. Chem.*, 1981, **34**, 383 (*synth, pmr*)
Sinhababu, A.K. *et al*, *J.O.C.*, 1983, **48**, 2356 (*synth, ir, pmr*)
Liu, C. *et al*, *CA*, 1990, **113**, 55822b (*isol*)

6-Methyl-1-hepten-4-ol M-1-00068

Allylisobutylcarbinol

[75863-15-9]



(*R*)-*form*

$C_8H_{16}O$ M 128.2

(R)-form [133379-16-5]

Liq. Bp 60-62°. $[\alpha]_D$ +17.6 (c, 3 in CH_2Cl_2).

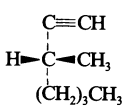
(±)-form

Liq. Bp_{748} 162-163°, Bp_{28} 95-100°.

Herrmann, R. *et al*, *Z. Naturforsch., B*, 1990, **45**, 1684 (*R-form*)
Imai, T. *et al*, *Synthesis*, 1993, 395 (*synth*)

3-Methyl-1-heptyne, 9CI M-1-00069

[53293-03-1]



(*R*)-*form*

C_8H_{14} M 110.1

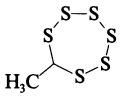
(R)-form [153219-25-1]
Oil. Bp 92-97°. $[\alpha]_D^{26}$ −25.3 (c, 1.7 in $CHCl_3$).

(±)-form
Liq. d_{20} 0.74. Bp 109-111°. n_D^{20} 1.4110.

Okhlobystin, O.Y. *et al*, *Neftekhimiya*, 1961, **1**, 752; *CA*, **57**, 14918f (*synth*)
Aoyagi, S. *et al*, *J.A.C.S.*, 1993, **115**, 11393 (*synth, ir, pmr, cmr*)

Methylhexathiepane M-1-00070

[151261-57-3]

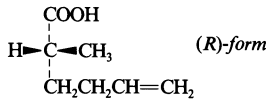


$C_2H_4S_6$ M 220.4
Prod. by *Thermococcus acidaminovorans* and *T. tadjuricus*.

Ritzau, M. *et al*, *Annalen*, 1993, 871.

2-Methyl-5-hexenoic acid M-1-00071

[77290-89-2]



(R)-form

$C_7H_{12}O_2$ M 128.1

(R)-form
Yellow oil. $[\alpha]_D^{25}$ −8.2 (c, 1.07 in CH_2Cl_2).

Benzyl ester: [135006-50-7].
$C_{14}H_{18}O_2$ M 218.2 $[\alpha]_D$ −11.3 (c, 2.89 in $CHCl_3$).

(±)-form
$Bp_{1.5}$ 120°.

Et ester: [86553-85-7].
$C_9H_{16}O_2$ M 156.2 Bp_{90} 103°.

Beckwith, A.L.J. *et al*, *Aust. J. Chem.*, 1983, **36**, 545 (*Et ester*)
Fujisawa, T. *et al*, *Tetrahedron*, 1989, **45**, 403 (*synth, pmr, ir*)
Wu, M.-J. *et al*, *Org. Prep. Proced. Int.*, 1994, **26**, 671 (*R-form, synth, cmr, pmr*)

2-Methyl-3-hexyne, 9CI M-1-00072

Ethylisopropylacetylene

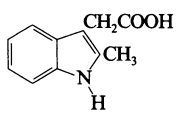
[36566-80-0]

$H_3CCH_2C{\equiv}CCH(CH_3)_2$

C_7H_{12} M 96.1
Liq. Bp 94-95°. n_D^{20} 1.4114.

Dedusenko, L.S., *CA*, 1943, **37**, 1697; 1944, **38**, 1466 (*synth*)
Levina, R.Ya. *et al*, *Zh. Obshch. Khim.*, 1956, **26**, 2195; *J. Gen. Chem. USSR (Engl. Transl.)*, 2453 (*synth*)
West, R. *et al*, *J.A.C.S.*, 1976, **98**, 8413 (*pmr, ir, ms*)
Mori, K. *et al*, *Annalen*, 1994, 817 (*synth*)

2-Methyl-1*H*-indole-3-acetic acid, 8CI M-1-00073



$C_{11}H_{11}NO_2$ M 189.2
Cryst. (MeOH). Mp 198°.

Me ester: [78564-10-0].
$C_{12}H_{13}NO_2$ M 203.2 Cryst. (petrol). Mp 67°.

Hydrazide: [21909-51-3].
Mp 164°.

Amide: [58360-14-8]. *2-Methyl-1H-indole-3-acetamide, 9CI*
$C_{11}H_{12}N_2O$ M 188.2 Cryst. Mp 96°.

Nitrile: [4071-16-3]. *2-Methyl-1H-indole-3-acetonitrile*
$C_{11}H_{10}N_2$ M 170.2 Cryst. (Et_2O). Mp 108-109°.

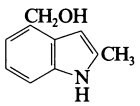
N-*Benzoyl:* [16401-80-2]. *1-Benzoyl-2-methyl-3-indoleacetic acid, 8CI.* ***Delmetacin, INN.*** *Demetacin. UR 2310*
$C_{18}H_{15}NO_3$ M 293.3 Analgesic, antipyretic, antiinflammatory agent. Mp 167-168°.
▶ LD_{50} (rat, orl) 362 mg/kg. LD_{50} (rat, ipr) 262 mg/kg. NL3350000.

Netherlands Pat., 6 605 169, (1966) (*Sumitomo*); *CA*, **67**, 90668j (*synth, pharmacol*)
Rimbau, V. *et al*, *Arch. Farmacol. Toxicol.*, 1982, **8**, 201 (*deriv, tox*)
Teuber, H.-J. *et al*, *Annalen*, 1983, 1744 (*synth*)

2-Methyl-1*H*-indole-4-methanol, 9CI M-1-00074

4-(Hydroxymethyl)-2-methyl-1H-indole

[154523-21-4]

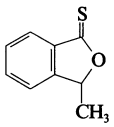


$C_{10}H_{11}NO$ M 161.2
Alkaloid from fruit bodies of the mushrooms *Tricholoma sciodes* and *T. virgatum*. Yellow oil.

Me ether: [154523-22-5]. ***4-(Methoxymethyl)-2-methylindole***
$C_{11}H_{13}NO$ M 175.2 From *T. sciodes* and *T. virgatum*. Yellow oil.

Garlaschelli, L. *et al*, *Tetrahedron*, 1994, **50**, 3571 (*isol, uv, ir, pmr, cmr, ms, struct*)

3-Methyl-1(3*H*)-isobenzofuranthione M-1-00075



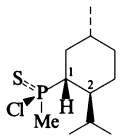
C_9H_8OS M 164.2

(±)-form
Cryst. Mp 61-63°. Bp_3 145°.

Nishio, T., *J.C.S. Perkin 1*, 1995, 561 (*synth, ir, pmr, cmr*)

Methyl (2-isopropyl-5-methylcyclohexyl) phosphinothioic chloride M-1-00076

Methyl[5-methyl-2-(1-methylethyl)cyclohexyl] phosphinothioic chloride, 9CI



(1R,2S,5R)-(Rp)-form

$C_{11}H_{22}ClPS$ M 252.7

(1R,2S,5R)-(R$_p$)-form [113613-11-9]
Menthylmethylphosphinothioic chloride. Menthylmethylthiophosphinic chloride
Obt. only as diastereisomer mixt.

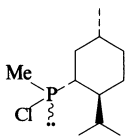
(1R,2S,5R)-(S$_p$)-form [113613-10-8]
Obt. 92% opt. pure. Solid. Mp 53°. Et, isopropyl, Ph and *tert*-butyl analogues also prepd. Cryst. struct. detn. is on the *tert*-butyl analogue.

[103633-99-4, 103634-00-0, 103953-56-6, 103953-57-7, 113613-12-0, 113613-13-1, 113613-14-2, 113613-15-3]

Boese, R. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1985, **25**, 103; 1986, **28**, 351 (*synth, pmr, P-31 nmr, cryst struct, analogues*)
Hägele, G. *et al*, *J.C.S. Dalton*, 1987, 795 (*synth, pmr, cmr, P-31 nmr*)

Methyl(2-isopropyl-5-methylcyclohexyl) phosphinous chloride, 8CI M-1-00077

Methyl[5-methyl-2-(1-methylethyl)cyclohexyl] phosphinous chloride, 9CI

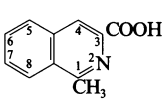


$C_{11}H_{22}ClP$ M 220.7

(1R,2S,5R)-form [92808-62-3]
Menthylmethylphosphinous chloride. Chloromethylmenthylphosphine
Liq. $Bp_{0.2-0.3}$ 78-80°. Epimers at P not recognisable spectroscopically because of rapid Cl exchange (distinction from Ph analogue (2-Isopropyl-5-methylcyclohexyl) phenylphosphinous chloride, I-1-00076).

Hägele, G. *et al*, *J.C.S. Dalton*, 1987, 795 (*synth, pmr, cmr, P-31 nmr*)

1-Methyl-3-isoquinolinecarboxylic acid, 9CI M-1-00078



$C_{11}H_9NO_2$ M 187.1

Me ester: [94726-23-5].
$C_{12}H_{11}NO_2$ M 201.2 Mp 104-105°.

Et ester: [86051-56-1].
$C_{13}H_{13}NO_2$ M 215.2 Mp 104°.

Hickey, D.M.B. *et al*, *J.C.S. Perkin 1*, 1986, 1113; 1987, 921 (*synth, ir, pmr, esters*)

1-Methyl-4-isoquinolinecarboxylic acid, 9CI M-1-00079

$C_{11}H_9NO_2$ M 187.1

Nitrile: [35005-95-9]. *4-Cyano-1-methylisoquinoline*
$C_{11}H_8N_2$ M 168.1 Needles (cyclohexane). Mp 100-101°.

[69230-00-8]

Taheuchi, I. *et al*, *Chem. Pharm. Bull.*, 1992, **40**, 2602 (*nitrile*)

3-Methyl-1-isoquinolinecarboxylic acid, 9CI M-1-00080

[105956-71-6]

$C_{11}H_9NO_2$ M 187.1

Nitrile: [22381-52-8]. *1-Cyano-3-methylisoquinoline*
$C_{11}H_8N_2$ M 168.1 Cryst. (petrol). Mp 105-106°.

Nitrile, 2-oxide: [16281-21-3].
$C_{11}H_8N_2O$ M 184.1 Mp 195-196°.

Kubo, A. *et al*, *Chem. Pharm. Bull.*, 1968, **16**, 1533 (*ms, nitrile*)
Simonsen, O. *et al*, *Acta Chem. Scand.*, 1970, **24**, 268 (*synth, nitrile, oxide*)
Kirby, G.W. *et al*, *J.C.S. Perkin 1*, 1979, 270 (*synth, ir, pmr, nitrile*)

3-Methyl-5-isoquinolinecarboxylic acid, 9CI M-1-00081

$C_{11}H_9NO_2$ M 187.1

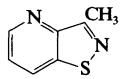
Nitrile:
$C_{11}H_8N_2$ M 168.1 Cryst. (petrol). Mp 127-129°.

[73459-97-9]

Elderfield, R.C. *et al*, *J.O.C.*, 1958, **23**, 435 (*synth, nitrile*)

3-Methylisothiazolo[4,5-*b*]pyridine M-1-00082

[147055-79-6]

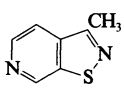


$C_7H_6N_2S$ M 150.2
Parent heterocycle currently unknown (1994). Cryst. with unpleasant odour. Mp 75-77°.

Chimichi, S. *et al*, *Synth. Commun.*, 1993, **23**, 73.

3-Methylisothiazolo[5,4-*c*]pyridine M-1-00083

[42242-20-6]



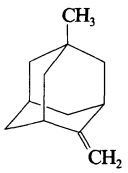
$C_7H_6N_2S$ M 150.2
Parent heterocycle currently unknown (1994). Pale orange solid. Mp 57-58°.

Taurins, A. *et al*, *Can. J. Chem.*, 1973, **51**, 1741 (*synth, pmr, uv*)
Chimichi, S. *et al*, *Synth. Commun.*, 1993, **23**, 73 (*synth*)

1-Methyl-4-methyleneadamantane M-1-00084

1-Methyl-4-methylenetricyclo[3.3.1.1^{3,7}]decane, 9CI

[155396-29-5]



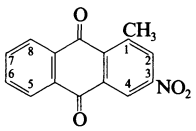
$C_{12}H_{18}$ M 162.2
Oil.

Adcock, W. *et al*, *J.O.C.*, 1994, **59**, 1867 (*synth, pmr, cmr*)

1-Methyl-3-nitroanthraquinone M-1-00085

1-Methyl-3-nitro-9,10-anthracenedione, 9CI

[92424-69-6]



$C_{15}H_9NO_4$ M 267.2
Yellow cryst. Mp 260-261.5°.

Gudzenko, V.I., *Zh. Obshch. Khim.*, 1963, **33**, 940; *CA*, **59**, 9925a (*synth*)

1-Methyl-4-nitroanthraquinone M-1-00086

1-Methyl-4-nitro-9,10-anthracenedione, 9CI

[42431-35-6]

$C_{15}H_9NO_4$ M 267.2
Mp 261-261.5°.

Fain, V.Ya. *et al*, *Zh. Obshch. Khim.*, 1961, **31**, 1588; *CA*, **55**, 24699q (*synth*)

1-Methyl-5-nitroanthraquinone M-1-00087

1-Methyl-5-nitro-9,10-anthracenedione, 9CI

[5025-16-1]

$C_{15}H_9NO_4$ M 267.2
Yellow needles (C_6H_6). Mp 254-256°.

Oda, N. *et al*, *Chem. Pharm. Bull.*, 1978, **26**, 2578 (*synth, ir*)

1-Methyl-8-nitroanthraquinone M-1-00088

1-Methyl-8-nitro-9,10-anthracenedione, 9CI

[5025-17-2]

$C_{15}H_9NO_4$ M 267.2
Yellow needles. Mp 258-260°.

Oda, N. *et al*, *Chem. Pharm. Bull.*, 1978, **26**, 2578 (*synth, ir*)

2-Methyl-1-nitroanthraquinone M-1-00089

2-Methyl-1-nitro-9,10-anthracenedione, 9CI

[129-15-7]

$C_{15}H_9NO_4$ M 267.2
Yellow cryst. (AcOH). Mp 272-273°.

▶ Suspected carcinogen.

Locher, A. *et al*, *Helv. Chim. Acta*, 1927, **10**, 642 (*synth*)
Wood, G.D. *et al*, *J.C.S.*, 1962, 3373 (*synth*)
Kim, J.I. *et al*, *J.A.C.S.*, 1992, **114**, 9309 (*pmr*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MMG000.

6-Methyl-1-nitroanthraquinone M-1-00090

6-Methyl-1-nitro-9,10-anthracenedione, 9CI

[68449-97-8]

$C_{15}H_9NO_4$ M 267.2
Yellow needles (C_6H_6). Mp 266°.

Oda, N. *et al*, *Chem. Pharm. Bull.*, 1978, **26**, 2578 (*synth, ir*)

7-Methyl-1-nitroanthroquinone M-1-00091

7-Methyl-1-nitro-9,10-anthracenedione, 9CI

[68449-99-0]

$C_{15}H_9NO_4$ M 267.2
Cryst. Mp 240-242°.

Oda, N. *et al*, *Chem. Pharm. Bull.*, 1978, **26**, 2578 (*synth, ir*)

(1-Methyl-1-nitroethyl)phosphonic acid M-1-00092

$O_2NC(CH_3)_2P(O)(OH)_2$

$C_3H_8NO_5P$ M 169.0
Solid (as anilinium salt). Mp 178° (anilinium salt).

Di-Me ester: [53753-43-8]. *Dimethyl (1-methyl-1-nitroethyl)phosphonate*
$C_5H_{12}NO_5P$ M 197.1 Liq. Mp 178° (anilinium salt). Bp_2 95-96°, $Bp_{0.1}$ 80-81°. n_D^{20} 1.4459.

Di-Et ester: [60171-51-9]. *Diethyl (1-methyl-1-nitroethyl)phosphonate*
$C_7H_{16}NO_5P$ M 225.1 Liq. Bp_2 107°. n_D^{20} 1.4357.

Dipropyl ester: [60171-52-0]. *Dipropyl (1-methyl-1-nitroethyl)phosphonate*
$C_9H_{20}NO_5P$ M 253.2 Liq. Bp_3 105°. n_D^{20} 1.4442.

Dichloride: [60171-57-5].
$C_3H_6Cl_2NO_3P$ M 205.9 Solid. Mp 128°.

[60171-54-2]

Petrov, K.A. *et al*, *Zh. Obshch. Khim.*, 1974, **44**, 1649; 1976, **46**, 1246; *J. Gen. Chem. USSR (Engl. Transl.)*, 1974, **44**, 1617; 1976, **46**, 1226 (*synth, esters*)
Russell, G.A. *et al*, *J.O.C.*, 1982, **47**, 1480 (*esters, synth, ir, ms, pmr, cmr, P-31 nmr*)

(1-Methyl-2-nitroethyl)phosphonic acid M-1-00093

$O_2NCH_2CH(CH_3)P(O)(OH)_2$

$C_3H_8NO_5P$ M 169.0
(±)-*form*

Di-Me ester: [56373-69-4]. *Dimethyl (1-methyl-2-nitroethyl)phosphonate*
$C_5H_{12}NO_5P$ M 197.1 Liq. $Bp_{0.2}$ 102°.

Di-Et ester: [42591-64-0]. *Diethyl (1-methyl-2-nitroethyl)phosphonate*
$C_7H_{16}NO_5P$ M 225.1 Liq. d_4^{20} 1.16. Bp_1 96-97°. n_D^{20} 1.4420.

Diisopropyl ester: [42591-65-1]. *Diisopropyl (1-methyl-2-nitroethyl)phosphonate*
$C_9H_{20}NO_5P$ M 253.2 Liq. d_4^{20} 1.10. Bp_1 86-87°. n_D^{20} 1.4385.

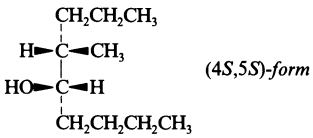
Dichloride:
$C_3H_6Cl_2NO_3P$ M 205.9 Liq. $Bp_{0.5}$ 78°. n_D^{20} 1.4940.

Lazareva, M.V. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1973, 1382; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1973, 1342 (*esters*)
Petrov, K.A. *et al, Zh. Obshch. Khim.*, 1976, **46**, 1246; *J. Gen. Chem. USSR (Engl. Transl.)*, 1976, **46**, 1226 (*esters, dichloride*)
Gareev, R.D. *et al, Zh. Obshch. Khim.*, 1978, **48**, 276; *J. Gen. Chem. USSR (Engl. Transl.)*, 1978, **48**, 245 (*di-Et ester, synth, ir, pmr*)
Yamashita, M. *et al, Synthesis*, 1987, 62 (*Di-Me ester*)

4-Methyl-5-nonanol M-1-00094

Ferrugineol. *Rhynchophorol III*

[154170-44-2]



(4*S*,5*S*)-*form*

$C_{10}H_{22}O$ M 158.2

(***4S,5S*)-*form*** [155073-31-7]
Aggregation pheromone from the male *Rhynchophorus ferrugineus* and *R. vulneratus*. Bp_{26} 80-89°. $[\alpha]_D^{19}$ −26.5 (c, 0.88 in Et_2O). n_D^{18} 1.4383. (4*R*,5*R*)-enantiomer also synthesised.

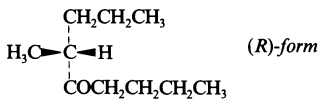
[152045-16-4, 152783-91-0, 155073-30-6]

Mori, K. *et al, Annalen*, 1993, 1201 (*synth, ir, pmr, cmr*)
Rochat, D. *et al, C. R. Hebd. Seances Acad. Sci. Ser. 2*, 1993, **316**, 1737 (*isol*)
Hallett, R.H. *et al, Naturwissenschaften*, 1993, **80**, 328 (*isol*)

4-Methyl-5-nonanone M-1-00095

Ferrugineone

[35900-26-6]



(*R*)-*form*

$C_{10}H_{20}O$ M 156.2
Aggregation pheromone of the palm weevils *Rhynchophorus* spp. Abs. config. of nat. prod. was not determined.

(***R*)-*form*** [67410-09-7]
Liq. Bp_{13} 130°. $[\alpha]_D$ −17.7 (c, 2.6 in Et_2O).

(***S*)-*form*** [77858-10-7]
$[\alpha]_D^{23}$ +14.8 (c, 3 in Et_2O).

(±)-*form*
Bp 189-190°.

Kletzke, P.G., *J.O.C.*, 1964, **29**, 1363 (*synth*)
Posner, G.H. *et al, J.A.C.S.*, 1973, **95**, 3076 (*synth*)
Amos, R.A. *et al, J.O.C.*, 1977, **42**, 2537 (*synth, pmr*)
Meyers, A.I. *et al, J.A.C.S.*, 1981, **103**, 3088 (*synth*)
Enders, D. *et al, Tetrahedron*, 1984, **40**, 1345 (*synth, ir, pmr*)
Hallett, R.H. *et al, Naturwissenschaften*, 1993, **80**, 328 (*isol*)

2-Methyl-2-octanol, 9CI M-1-00096

[628-44-4]

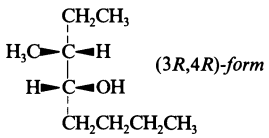
$H_3C(CH_2)_5C(CH_3)_2OH$

$C_9H_{20}O$ M 144.2
Liq. Bp 178°, $Bp_{7.5}$ 55°. n_D^{20} 1.4281.

Tarasova, G.A. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1956, 1267; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1956, 1297 (*synth*)
Herbertz, T., *Chem. Ber.*, 1959, **92**, 541 (*synth*)
Sowinski, A.F. *et al, J.O.C.*, 1979, **44**, 2369 (*synth, ms*)
Novak, M. *et al, J. Chem. Educ.*, 1993, **70**, A103 (*synth, pmr, cmr*)
Kiehl, A. *et al, Annalen*, 1995, 223 (*synth, pmr, cmr*)

3-Methyl-4-octanol M-1-00097

[26533-35-7]



(3*R*,4*R*)-*form*

$C_9H_{20}O$ M 144.2

(***3R,4R*)-*form*** [151765-86-5]
Bp_{24} 70-76°. $[\alpha]_D^{19}$ +20.3 (c, 1.05 in Et_2O). n_D^{20} 1.4334.

(***3S,4S*)-*form*** [151765-88-7] ***Rhynchophorol II***
Aggregation pheromone of the male *Rhynchophorus phoenicis*. Bp_{34} 84-92°. $[\alpha]_D^{20}$ −20.7 (c, 1.01 in Et_2O). n_D^{19} 1.4336.

(***3RS,4RS*)-*form*** [151698-74-7]
Bp_{27} 80-85°. n_D^{19} 1.4344.

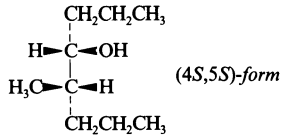
(***3RS,4SR*)-*form*** [151698-76-9]
Bp_{28} 74-80°. n_D^{19} 1.4348.

[98612-11-4, 98612-12-5]

Undavia, N.K. *et al, J. Inst. Chem. (India)*, 1974, **46**, 156 (*synth*)
Yamamoto, Y. *et al, J.A.C.S.*, 1985, **107**, 6411 (*synth*)
Mori, K. *et al, Annalen*, 1993, 865 (*synth, abs config, pmr*)
Gries, G. *et al, Naturwissenschaften*, 1993, **80**, 90 (*isol*)

5-Methyl-4-octanol, 9CI M-1-00098

[59734-23-5]



(4*S*,5*S*)-*form*

$C_9H_{20}O$ M 144.2

(***4S,5S*)-*form*** [154802-25-2] ***Cruentol***
Aggregation pheromone of the palmetto weevil *Rhynchophorus cruentatus*. Liq. Bp_{32} 82-84°. $[\alpha]_D^{19}$ −33.1 (c, 1.1 in Et_2O) (99.3% ee).

(±)-*form*
Liq. Bp_9 74-76°. Prob. mixt. of stereoisomers.

Bjelouss, E., *Ber.*, 1912, **45**, 625 (*synth*)
LeBel, N.A. *et al, J.O.C.*, 1963, **28**, 615 (*synth*)
Pinazzi, C. *et al, Bull. Soc. Chim. Fr.*, 1971, 1008; 1976, 501 (*synth, pmr*)
Perez, A.L. *et al, J. Chem. Ecol.*, 1994, **20**, 505, 2653 (*synth, pmr, cmr, ms*)
Mork, K. *et al, Annalen*, 1995, 697 (*cruentol, ir, pmr, cmr, ms*)

7-Methyl-4-octanol, 9CI M-1-00099

Isobutylpropylcarbinol

[33933-77-6]

$(H_3C)_2CHCH_2CH_2CH(OH)CH_2CH_2CH_3$

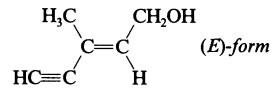
$C_9H_{20}O$ M 144.2

(±)-*form*
Liq. Bp 184-186°, Bp_{18} 89°. n_D^{20} 1.4260.

Thoms, H. *et al, Arch. Pharm. (Weinheim, Ger.)*, 1925, **263**, 241 (*synth*)
Tuot, M., *C. R. Hebd. Seances Acad. Sci.*, 1936, **202**, 1339 (*synth*)
Roscher, N.M. *et al, Tetrahedron*, 1984, **40**, 2643 (*ir, pmr*)

3-Methyl-2-penten-4-yn-1-ol M-1-00100

[105-29-3]



(*E*)-*form*

C_6H_8O M 96.1

(***E*)-*form*** [6153-05-5]
Liq. d 0.92. Bp 165-167°.

Formyl: [132992-60-0].
$C_7H_8O_2$ M 124.1 Liq. Bp_5 71°.

Ac: [35272-88-9].
$C_8H_{10}O_2$ M 138.1 Liq. Bp_5 72°.

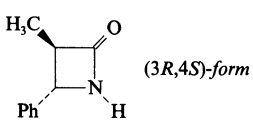
(***Z*)-*form*** [6153-06-6]
Liq. d 0.90. Bp_{30} 89-92°. n_D^{20} 1.4930.

Formyl: [132992-59-7].
Liq. Bp_5 62°.

Ac: [35272-87-8].
Liq. Bp_5 65°.

Cymerman, J. *et al, J.C.S.*, 1945, 90 (*synth*)
Oroshnik, W., *J.A.C.S.*, 1956, **78**, 2651 (*synth*)
Mori, K. *et al, Tetrahedron*, 1972, **28**, 3739 (*synth, bibl, ir, pmr*)
Bader, H. *et al, Chem. Ber.*, 1989, **122**, 1193 (*synth, Ac, pmr, cmr, ir*)
Zacharias, M.T. *et al, Indian J. Chem., Sect. B*, 1991, **30**, 59 (*synth, Ac, ir, pmr*)

3-Methyl-4-phenyl-2-azetidinone M-1-00101



(3*R*,4*S*)-*form*

$C_{10}H_{11}NO$ M 161.2

(***3R,4S*)-*form*** [151214-59-4]
$[\alpha]_D^{25}$ −39.0 (c, 1.00 in $CHCl_3$).

(*3S,4S*)-*form* [151214-62-9]
$[\alpha]_D^{25}$ −206.7 (c, 1.04 in $CHCl_3$).

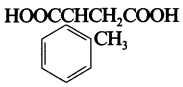
(*3RS,4RS*)-*form* [16934-12-6]
(±)-cis-*form*
Cryst. Mp 105.6°.

(*3RS,4SR*)-*form* [16934-13-7]
(±)-trans-*form*
Cryst. Mp 99-100°.

Moriconi, E.J. *et al*, *Tet. Lett.*, 1968, 1435 (*synth*)
Durst, T. *et al*, *Can. J. Chem.*, 1974, **52**, 3206 (*synth*)
Yamamoto, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 319 (*synth, pmr, cmr*)
Davies, S.G. *et al*, *Chem. Comm.*, 1993, 1153 (*synth*)

(2-Methylphenyl)butanedioic acid, 9CI M-1-00102

o-*Tolylsuccinic acid*



$C_{11}H_{12}O_4$ M 208.2

(±)-*form*
Prisms (EtOH aq.); plates (H_2O). Mp 184-185° (181-182°), Mp 204-205°.

Di-Me ester: [37741-55-2].
$C_{13}H_{16}O_4$ M 236.2 Liq. $Bp_{0.2}$ 140°.

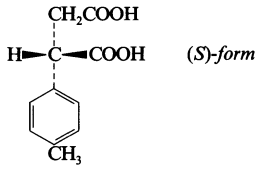
Anhydride:
$C_{11}H_{10}O_3$ M 190.1 Waxy prisms (Et_2O). Mp 45-46°. Bp_5 174-176°.

Alder, K. *et al*, *Annalen*, 1949, **565**, 99 (*synth*)
Potts, K.T. *et al*, *J.C.S.*, 1955, 2466 (*synth*)
Mori, K. *et al*, *Agric. Biol. Chem.*, 1963, **27**, 27 (*synth*)
House, H.O. *et al*, *J.O.C.*, 1973, **38**, 741 (*synth, anhydride, di-Me ester*)

(4-Methylphenyl)butanedioic acid, 9CI M-1-00103

p-*Tolylsuccinic acid*

[66483-40-7]



(*S*)-*form*

$C_{11}H_{12}O_4$ M 208.2

(*S*)-*form* [89359-07-9]
Mp 204-206°. $[\alpha]_D^{21}$ +160 (c, 1.4 in Me_2CO).

(±)-*form*
Cryst. (H_2O). Mp 210°.

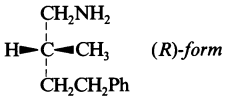
Di-Me ester: [36265-44-8].
$C_{13}H_{16}O_4$ M 236.2 Liq. $Bp_{0.2}$ 119-121°.

Alder, K. *et al*, *Annalen*, 1949, **565**, 99 (*synth*)
Lawston, I.W. *et al*, *J.C.S. Perkin 1*, 1983, 2629 (*synth*)
Taylor, E.C. *et al*, *J.O.C.*, 1984, **49**, 3840 (*di-Me ester*)
Rossi, E. *et al*, *Synthesis*, 1986, 765 (*synth*)
Marwah, A.K. *et al*, *Synth. Commun.*, 1995, **25**, 235 (*synth, ir, pmr*)

2-Methyl-4-phenyl-1-butylamine M-1-00104

β-Methylbenzenebutanamine, 9CI

[65476-99-5]



(*R*)-*form*

$C_{11}H_{17}N$ M 163.2

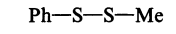
(*R*)-*form* [142363-25-5]
$[\alpha]_D^{20}$ +12.4 (c, 2.0 in $CHCl_3$) (*ca.* 80% ee).

(±)-*form*
Oil. $Bp_{0.2}$ 105°.

Reissig, H.-U. *et al*, *Annalen*, 1990, 475; 1995, 667 (*synth, pmr, ir*)
Arnold, T. *et al*, *Angew. Chem.*, 1992, **104**, 1084 (*R-form*)

Methyl phenyl disulfide M-1-00105

[14173-25-2]



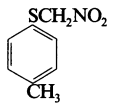
$C_7H_8S_2$ M 156.2
Liq. $Bp_{0.5}$ 86°. n_D^{25} 1.6135.

Armitage, D.A. *et al*, *J.C.S. Perkin 1*, 1972, 680 (*synth, pmr*)
Capozzi, G. *et al*, *Gazz. Chim. Ital.*, 1990, **120**, 421 (*synth, pmr, ms*)
Metzner, P. *et al*, *Synthesis*, 1994, 761 (*synth, pmr, cmr, ms*)

4-Methylphenyl nitromethyl sulfide M-1-00106

1-Methyl-4-(nitromethylthio)benzene, 9CI. Nitromethyl p-*tolyl sulfide*

[150640-22-5]



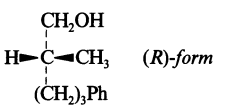
$C_8H_9NO_2S$ M 183.2
No phys. props. reported.

S,S-*Dioxide:* [51351-89-4]. *4-Methylphenyl nitromethyl sulfone. 1-Methyl-4-[(nitromethyl)sulfonyl]benzene, 9CI. Nitromethyl* p-*tolyl sulfone*
$C_8H_9NO_4S$ M 215.2 Mp 115-116.5°.

Langler, R.F. *et al*, *Aust. J. Chem.*, 1994, **47**, 1641.

2-Methyl-5-phenyl-1-pentanol M-1-00107

β-Methylbenzenepentanol, 9CI



(*R*)-*form*

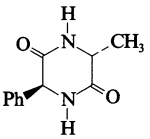
$C_{12}H_{18}O$ M 178.2

(*R*)-*form* [156767-44-1]
Oil. $[\alpha]_D^{25}$ +11.2 (c, 6.6 in EtOH).

Santini, C. *et al*, *J.O.C.*, 1994, **59**, 2261 (*synth, pmr, cmr, ir, ms*)

3-Methyl-6-phenyl-2,5-piperazinedione, 9CI M-1-00108

Cyclo(alanylphenylglycine)



(3*R*,6*S*)-*form*

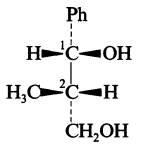
$C_{11}H_{12}N_2O_2$ M 204.2
Anticonvulsant.

(*3R,6S*)-*form* [35590-99-9]
Cryst.

[35590-98-8]

Westley, J.W. *et al*, *Anal. Chem.*, 1968, **40**, 1888 (*synth, pmr*)
Slater, G.P. *et al*, *J. Chromatogr.*, 1972, **64**, 166 (*glc*)
Szkaradzinska, M.B. *et al*, *Acta Cryst. C*, 1994, **50**, 565 (*cryst struct*)

2-Methyl-1-phenyl-1,3-propanediol, 9CI M-1-00109



(1*R*,2*S*)-*form*

$C_{10}H_{14}O_2$ M 166.2

(*1R,2S*)-*form*
(+)-erythro-*form*
Cryst. (Et_2O/hexane). Mp 75-76°. $[\alpha]_D^{20}$ +57.8 (c, 0.45 in $CHCl_3$).

(*1S,2R*)-*form* [127379-92-4]
(−)-erythro-*form*
Flakes. Mp 74-75°. $[\alpha]_D^{22}$ −62.5 (c, 0.48 in $CHCl_3$).

(*1RS,2RS*)-*form* [7087-77-6]
(±)-erythro-*form*
Liq.

(*1RS,2SR*)-*form* [14366-91-7]
(±)-threo-*form*
Liq.

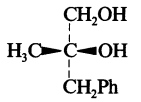
Bis(p-*nitrobenzoyl*): Pale yellow prisms (C_6H_6). Mp 156-157°.

[51451-31-1, 51451-32-2, 139068-60-3]

Koga, K. *et al*, *Chem. Pharm. Bull.*, 1972, **20**, 526 (*synth, pmr*)
Balsano, A. *et al*, *J.O.C.*, 1975, **40**, 473 (*synth*)
Oppolzer, W. *et al*, *J.A.C.S.*, 1990, **112**, 2767 (*synth*)
Banks, M.R. *et al*, *Chem. Comm.*, 1993, 1146 (*synth*)

2-Methyl-3-phenyl-1,2-propanediol, 9CI M-1-00110

[90926-14-0]



(*R*)-*form*

$C_{10}H_{14}O_2$ M 166.2

(*R*)-*form* [96948-92-4]
Cryst. (pentane/Et_2O). Mp 66.5-67.5°. $[\alpha]_D^{20}$ +17.3 (c, 1.1 in EtOH aq.) (*ca.* 95% ee).

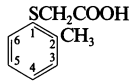
(±)-*form* [96998-28-6]
Needles (Et_2O/cyclohexane). Sol. H_2O. Mp 55-56°.

Davies, A.G. *et al*, *J.C.S.*, 1957, 3154 (*synth, resoln*)
Frye, S.V. *et al*, *J.O.C.*, 1985, **50**, 3402 (*asymm synth, pmr, cmr*)
Tamura, Y. *et al*, *Chem. Pharm. Bull.*, 1987, **35**, 4736 (*asymm synth*)
Bach, T., *Annalen*, 1995, 1045 (*synth, ir, pmr, cmr, ms*)

[(2-Methylphenyl)thio]acetic acid, 9CI M-1-00111

(o-*Tolylthio*)*acetic acid, 8CI.* o-*Tolylthioglycolic acid*

[18619-15-3]



$C_9H_{10}O_2S$ M 182.2
Cryst. (H_2O). Mp 108-109°.

S-*Oxide*, (R)-: [125982-97-0]. [(*2-Methylphenyl*)*sulfinyl*]*acetic acid, 9CI*
$C_9H_{10}O_3S$ M 198.2 Mp 85-88°. $[\alpha]_D$ +93.0 (CH_2Cl_2).

Behagel, O. *et al*, *J. Prakt. Chem.*, 1926, **114**, 287 (*synth*)
Oksengendler, G.M. *et al*, *Zh. Obshch. Khim.*, 1957, **27**, 3214; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1957, **27**, 3251 (*synth*)
Drabowicz, J. *et al*, *Croat. Chem. Acta*, 1989, **62**, 423 (*S-oxide*)
Yildirir, Y. *et al*, *Org. Prep. Proced. Int.*, 1995, **27**, 381 (*synth, pmr*)

[(3-Methylphenyl)thio]acetic acid, 9CI M-1-00112

(m-*Tolylthio*)*acetic acid, 8CI.* m-*Tolylthioglycolic acid*

[3996-30-3]

$C_9H_{10}O_2S$ M 182.2
Needles (C_6H_6/petrol). Mp 67.5-68.0°, Mp 104°. pK_a 3.60 (25°, H_2O).

Et ester: [14738-26-2].
$C_{11}H_{14}O_2S$ M 210.2 Bp_1 120°.

Nitrile: [16798-95-1]. (m-*Tolylthio*)*acetonitrile, 8CI*
C_9H_9NS M 163.2 Bp_1 119°.

S-*Oxide*, (R)-: [125982-96-9]. [(*3-Methylphenyl*)*sulfinyl*]*acetic acid, 9CI*
$C_9H_{10}O_3S$ M 198.2 Mp 86-90°. $[\alpha]_D$ +35.0 (CH_2Cl_2).

S,S-*Dioxide:* (m-*Tolylsulfonyl*)*acetic acid*
$C_9H_{10}O_4S$ M 214.2 Mp 85-85.5°.

Behagel, O. *et al*, *J. Prakt. Chem.*, 1926, **114**, 287 (*synth*)
Tarbell, D.S. *et al*, *J.A.C.S.*, 1946, **68**, 1456 (*synth*)
Oksengendler, G.M. *et al*, *Zh. Obshch. Khim.*, 1957, **27**, 3214; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1957, **27**, 3251 (*synth*)
Ishida, S. *et al*, *Agric. Biol. Chem.*, 1967, **31**, 651 (*nitrile, Et ester*)
Drabowicz, J. *et al*, *Croat. Chem. Acta*, 1989, **62**, 423 (*S-oxide*)
Cabiddu, S. *et al*, *Tetrahedron*, 1990, **46**, 861 (*synth*)

[(4-Methylphenyl)thio]acetic acid, 9CI M-1-00113

(p-*Tolylthio*)*acetic acid, 8CI.* p-*Tolylthioglycolic acid*

[3996-29-0]

$C_9H_{10}O_2S$ M 182.2
Cryst. (hexane/toluene). Mp 95-97° (88-90°). pK_a 3.96 (25°, H_2O).

Et ester: [14738-27-3].
$C_{11}H_{14}O_2S$ M 210.2 Pale yellow liq. Bp_{14} 157°.

Nitrile: [21681-88-9].
C_9H_9NS M 163.2 Bp_3 168-170°.

Nitrile, S,S-*dioxide:* [5697-44-9]. p-*Toluenesulfonylacetonitrile.* p-*Tosylacetonitrile*
$C_9H_9NO_2S$ M 195.2 Cryst. (MeOH or C_6H_6). Mp 149-150°.

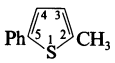
S-*Oxide* (R-): [88981-65-1]. [(*4-Methylphenyl*)*sulfinyl*]*acetic acid, 9CI*
$C_9H_{10}O_3S$ M 198.2 Cryst. (EtOAc/hexane). Mp 105-106°. $[\alpha]_D^{25}$ +192.4 (c, 11.8 in Me_2CO).

S,S-*Dioxide:* [3937-96-0]. [(*4-Methylphenyl*)*sulfonyl*]*acetic acid, 9CI.* (p-*Tolylsulfonyl*)*acetic acid, 8CI*
$C_9H_{10}O_4S$ M 214.2 Cryst. (CH_2Cl_2). Mp 114-115°.

Behagel, O. *et al*, *J. Prakt. Chem.*, 1926, **114**, 287 (*synth*)
Müller, E. *et al*, *J. Prakt. Chem.*, 1936, **146**, 56 (*synth, Et ester*)
Oksengendler, G.M. *et al*, *Zh. Obshch. Khim.*, 1957, **27**, 3214; *J. Gen. Chem. USSR* (*Engl. Transl.*), 3251 (*synth*)
Meek, J.S. *et al*, *J.O.C.*, 1968, **33**, 3418 (*tosylacetonitrile*)
Magnus, P. *et al*, *J.A.C.S.*, 1984, **106**, 2105 (*S-oxide*)
Sepiol, J.J. *et al*, *J.O.C.*, 1984, **49**, 1125 (*tosylacetonitrile*)
Gupton, J.T. *et al*, *J.O.C.*, 1991, **56**, 976 (*S,S-dioxide*)
Yildirir, Y. *et al*, *Org. Prep. Proced. Int.*, 1995, **27**, 381 (*synth, pmr*)

2-Methyl-5-phenylthiophene, 9CI M-1-00114

[5069-26-1]



$C_{11}H_{10}S$ M 174.2
Mp 49-51°.

Voronkov, M.G. *et al*, *Zh. Obshch. Khim.*, 1950, **20**, 1218; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1950, **20**, 1263 (*synth*)
Duus, F., *Tetrahedron*, 1976, **32**, 2817 (*synth*)
Shridasar, D.R. *et al*, *Synthesis*, 1982, 1061 (*synth, pmr*)
Kharchenko, V.G. *et al*, *Khim. Geterotsikl. Soedin.*, 1984, 1606; *Chem. Heterocycl. Compd.* (*Engl. Transl.*), 1984, 1321 (*synth, pmr*)
Freeman, F. *et al*, *J.O.C.*, 1992, **57**, 1722 (*synth, pmr, cmr*)

3-Methyl-2-phenylthiophene, 9CI M-1-00115

[14300-30-2]

$C_{11}H_{10}S$ M 174.2
Oil. Bp 257-258.7°, Bp_{16} 135°. n_D^{20} 1.6209.

Voronkov, M.G. *et al*, *Zh. Obshch. Khim.*, 1950, **20**, 1218; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1950, **20**, 1263 (*synth*)
Cagniant, P. *et al*, *C. R. Hebd. Seances Acad. Sci. Ser. C*, 1975, **281**, 35 (*synth*)
Kang, K.-T. *et al*, *Synth. Commun.*, 1995, **25**, 2647 (*synth, pmr, cmr, ms*)

4-Methyl-2-phenylthiophene, 9CI M-1-00116

[14300-29-9]

$C_{11}H_{10}S$ M 174.2
Oil. Mp 17°. Bp_{773} 280°, Bp_5 115-120°.

Voronkov, M.G. *et al*, *Zh. Obshch. Khim.*, 1950, **20**, 1218; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1950, **20**, 1263 (*synth*)
Tilak, B.D. *et al*, *Indian J. Chem.*, 1969, **7**, 9 (*synth, ir, uv*)
Campaigne, E. *et al*, *J. Het. Chem.*, 1988, **25**, 367 (*synth, ir, pmr*)

P,P'-[(Methylphosphinidene) di-2,1-ethanediyl]bis[*N,N,N',N'*-tetramethylphosphonous diamide] M-1-00117

[63578-31-4]

$MeP[CH_2CH_2P(NMe_2)_2]_2$

$C_{13}H_{35}N_4P_3$ M 340.3
Ligand. Liq. $Bp_{0.005}$ 130-133°.

King, R.B. *et al*, *J.A.C.S.*, 1977, **99**, 4001 (*synth, pmr, cmr, P-31 nmr*)

[(Methylphosphinylidene) dimethylene]diphosphonic acid, 8CI M-1-00118

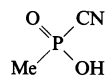
[(*Methylphosphinylidene*)*bis*(*methylene*)] *bisphosphonic acid*

$MeP(O)[CH_2P(O)(OH)_2]_2$

$C_3H_{11}O_7P_3$ M 252.0
Tri-p-*toluidine salt:* Solid. Mp 181-183°.
Tetra-Et ester: [18788-45-9]. *Tetraethyl* [(*methylphosphinylidene*)*dimethylene*] *diphosphonate. Tetraethyl* [(*methylphosphinylidene*)*bis*(*methylene*)] *bisphosphonate*
$C_{11}H_{27}O_7P_3$ M 364.2 Solid. Mp 99-101° (107°).

Medved', T.Ya., *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1968, 2062; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1968, 1959.
Maier, L. *et al*, *Helv. Chim. Acta*, 1969, **52**, 845 (*ester, synth, pmr, P-31 nmr*)

Methylphosphonocyanidic acid M-1-00119



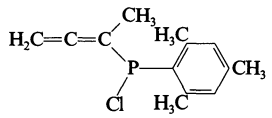
$C_2H_4NO_2P$ M 105.0
Me ester: [101153-04-2]. *Methyl methylphosphonocyanidate*
$C_3H_6NO_2P$ M 119.0 Liq. d_4^{20} 1.16. Bp_{13} 89-92°. n_D^{20} 1.4224.
Et ester: [117889-37-9]. *Ethyl methylphosphonocyanidate*
$C_4H_8NO_2P$ M 133.0 Liq. d_4^{20} 1.11. Bp_1 60-62°. n_D^{20} 1.4217.

Isopropyl ester: Isopropyl methylphosphonocyanidate
$C_5H_{10}NO_2P$ M 147.1 Liq. d_4^{20} 1.06. Bp_{5-6} 83-84°. n_D^{20} 1.4216.

Petrov, K.A. *et al*, *Zh. Obshch. Khim.*, 1959, **29**, 1827 (*synth*)
Krolevets, A.A. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1992, 187; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1992, 153.

(1-Methylpropadienyl)(2,4,6-trimethylphenyl)phosphinous chloride M-1-00120

Mesityl(1-methylallenyl)phosphinous chloride
[137787-52-1]



$C_{13}H_{16}ClP$ M 238.6
Air-sensitive, yellow oil. $Bp_{0.1}$ 170° (oven).

Nief, F. *et al*, *Tetrahedron*, 1991, **47**, 6673 (*synth, pmr, cmr, P-31 nmr*)

2-Methyl-2-propenethioic acid, 9CI M-1-00121

2-Methylthioacrylic acid, 8CI. Thiomethacrylic acid

$H_2C{=}C(CH_3)COSH$

C_4H_6OS M 102.1
S-*Me ester:* [52496-39-6].
C_5H_8OS M 116.1 Yellow oil. Bp_{36} 58°.
S-*Et ester:* [54667-15-1].
$C_6H_{10}OS$ M 130.2 Yellow liq. Bp_{42} 75°, Bp_{13} 50-51°.
S-*Ph ester:* [54667-28-6].
$C_{10}H_{10}OS$ M 178.2 Liq. Bp_3 103-104°.

Braude, G., *J.O.C.*, 1957, **22**, 1675 (*synth, esters*)
Sumrell, G. *et al*, *J.A.C.S.*, 1958, **80**, 2509 (*synth, esters*)
Wladislaw, B. *et al*, *Synth. Commun.*, 1990, **20**, 2937 (*ir, pmr, Me ester*)
Cerf, M. *et al*, *Sulfur Lett.*, 1992, **15**, 147 (*synth, ester*)

1-Methyl-3-(2-propenyl) benzene, 9CI M-1-00122

m-*Allyltoluene, 8CI. 3-(3-Methylphenyl) propene. 3-*m*-Tolylpropene. 1-Allyl-3-methylbenzene*
[3333-20-8]
$C_{10}H_{12}$ M 132.2
Liq. $Bp_{0.05}$ 24-27°.

Breen, P.J. *et al*, *J. Phys. Chem.*, 1989, **93**, 6731 (*synth, pmr, cmr*)

P-(2-Methyl-1-propenyl) phosphonous diamide M-1-00123

Isobutenylphosphonous diamide

$(H_3C)_2C{=}CHP(NH_2)_2$

$C_4H_{11}N_2P$ M 118.1
N,N,N′,N′-*Tetra-Me:* [72256-59-8].
N,N,N′,N′-*Tetramethyl*-P-(*2-methyl-1-propenyl*)*phosphonous diamide*
$C_8H_{19}N_2P$ M 174.2 Liq. Bp_{10} 77-79.5°.
N,N,N′,N′-*Tetra-Et:* [103794-52-1].
N,N,N′,N′-*Tetraethyl*-P-(*2-methyl-1-propenyl*)*phosphonous diamide*
$C_{12}H_{27}N_2P$ M 230.3 Liq. d_4^{20} 0.91. $Bp_{0.045}$ 62°. n_D^{20} 1.4886.

Baban, J.A. *et al*, *J.C.S. Perkin 2*, 1979, 781 (*tetramethyl*)
Pudonik, A.N. *et al*, *Zh. Obshch. Khim.*, 1985, **55**, 1479; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1985, **55**, 1316 (*tetraethyl*)

(2-Methylpropoxy)ethylene M-1-00124

Isobutyl vinyl ether. Ethenyl 2-methylpropyl ether
[109-53-5]

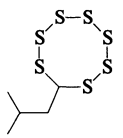
$(H_3C)_2CHCH_2OCH{=}CH_2$

$C_6H_{12}O$ M 100.1
d 0.77. Bp 82-84°. n_D^{20} 1.3970.

Schildknecht, C.F. *et al*, *Ind. Eng. Chem.*, 1947, **39**, 182.
Rowlands, D.C. *et al*, *J.O.C.*, 1952, **17**, 807.

(2-Methylpropyl) heptathiocane M-1-00125

Isobutylheptathiocane
[151261-59-5]

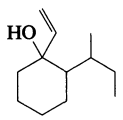


$C_5H_{10}S_7$ M 294.5
Prod. by *Thermococcus acidaminovorans* and *T. tadjuricus*. Pale yellow oil.

Ritzau, M. *et al*, *Annalen*, 1993, 871.

2-(1-Methylpropyl)-1-vinylcyclohexanol M-1-00126

1-Ethenyl-2-(1-methylpropyl)cyclohexanol
[37172-03-5]

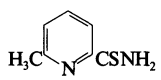


$C_{12}H_{22}O$ M 182.3
Ac: [37172-02-4]. *Dihydro ambrate*
$C_{14}H_{24}O_2$ M 224.3 Perfumery ingredient, fixative. Liq. with woody amber odour. d 0.95.

Ger. Pat., 2 155 671, (1972); *CA*, **77**, 61367m.

6-Methyl-2-pyridinecarbothioamide, 9CI M-1-00127

6-Methylthioicolinamide, 8CI
[5933-30-2]



$C_7H_8N_2S$ M 152.2
Used as 1 mM soln. in pentanol for extraction - photometric detn. of Cu(I) (λ_{max} 495 nm, in the presence of ascorbic acid). Cryst. pK_a 9.1 (H_2SO_4 aq. at 25°).

Walter, W. *et al*, *Annalen*, 1970, **733**, 170 (*synth, struct, ir*)
Tissier, C. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 3752; 1972, 2109 (*props*)
Wawschinek, O. *et al*, *J. Clin. Chem. Clin. Biochem.*, 1981, **19**, 541; *CA*, **95**, 128674b (*detn, Cu*)
Seko, N. *et al*, *Chem. Pharm. Bull.*, 1991, **39**, 651 (*synth*)

2-Methyl-4-pyrimidinecarboxylic acid M-1-00128

[13627-49-1]

$C_6H_6N_2O_2$ M 138.1
Cryst. (H_2O). Mp 203-206° dec.
Me ester: [73955-55-2].
$C_7H_8N_2O_2$ M 152.1 Mp 54-56°.
Nitrile: [64571-34-2]. *4-Cyano-2-methylpyrimidine*
$C_6H_5N_3$ M 119.1 Mp 29-30.5°. Bp_{15} 92-93°.

Reiner, R. *et al*, *Helv. Chim. Acta*, 1967, **50**, 128 (*synth, uv, pmr, ir*)
Yamanaka, H. *et al*, *Chem. Pharm. Bull.*, 1977, **25**, 1821 (*nitrile*)

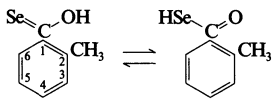
4-Methylpyrylium(1+) M-1-00129

$C_6H_7O^{\oplus}$ M 95.1 (ion)
Tetrafluoroborate: [162087-56-1].
$C_6H_7BF_4O$ M 181.9 Pale tan solid. Mp 111-114°. Rapidly darkens in air.

Taylor, R.J.K. *et al*, *J.C.S. Perkin 1*, 1995, 2385 (*synth, pmr, cmr*)

2-Methylselenobenzoic acid M-1-00130

2-Methylbenzenecarboselenoic acid, 9CI
[105223-25-4]



C_8H_8OSe M 199.1
Unstable oil. Dec. in air to diselenide.

OH-form

Amide: [93756-97-9].
C_8H_9NSe M 198.1 Yellow solid. Mp 104-106°.

SeH-form

Na salt: [135249-92-2].
Cryst. Mp 130-135° dec. Oxid. on standing in air.
Et ester: [135250-01-0].
$C_{10}H_{12}OSe$ M 227.1 Liq. $Bp_{0.2}$ 70°.

Sonoda, N. *et al*, *J.O.C.*, 1985, **50**, 384 (*amide*)
Kato, S. *et al*, *J. Prakt. Chem.*, 1990, **332**, 898 (*ester*)
Kato, S. *et al*, *J.A.C.S.*, 1994, **116**, 2195 (*synth, tautom*)

3-Methylselenobenzoic acid M-1-00131

3-Methylbenzenecarboselenoic acid

C_8H_8OSe M 199.1

OH-form

Amide: [68090-01-7].
C_8H_9NSe M 198.1 Yellow solid. Mp 84-85° (74°).

Cohen, V.I., *Synthesis*, 1978, 668 (*synth*)
Fan, W.-Q. *et al*, *Synth. Commun.*, 1994, **24**, 1761 (*synth, ir, pmr*)

4-Methylselenobenzoic acid M-1-00132

4-Methylbenzenecarboselenoic acid, 9CI

[105223-27-6]

C_8H_8OSe M 199.1
Unstable oil. Dec. in air to diselenide.

OH-form

Amide: [67213-27-8].
C_8H_9NSe M 198.1 Golden needles (EtOH). Mp 165-167° (161°), Mp 186°.

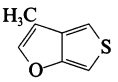
SeH-form

Na salt: [128816-64-8].
Cryst. Mp 135-145° dec. Oxid. on standing in air.

Et ester: [135250-02-1].
$C_{10}H_{12}OSe$ M 227.1 Liq. $Bp_{0.2}$ 66°.

Becker, W. *et al*, *Ber.*, 1904, **37**, 2550 (*amide*)
Cohen, V.I., *Synthesis*, 1978, 668 (*amide*)
Kato, S. *et al*, *J. Prakt. Chem.*, 1990, **332**, 898 (*ester*)
Reid, D.H. *et al*, *Synthesis*, 1993, 870 (*amide*)
Kato, S. *et al*, *J.A.C.S.*, 1994, **116**, 2195 (*synth, tautom*)
Fan, W.-Q. *et al*, *Synth. Commun.*, 1994, **24**, 1761 (*amide*)

3-Methylthieno[3,4-*b*]furan M-1-00133



C_7H_6OS M 138.1
$Bp_{0.1}$ 100°. Not obt. completely pure.

Buttery, J.H. *et al*, *Aust. J. Chem.*, 1995, **48**, 593 (*synth, pmr, cmr, ms*)

3-(Methylthio)-1,2-butadiene M-1-00134

[14044-71-4]

$H_2C{=}C{=}C(SMe)CH_3$

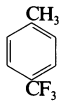
C_5H_8S M 100.1
Bp_{70} 60°.

Narasaka, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1992, **65**, 1392 (*synth, ir, ms, pmr, cmr*)

1-Methyl-4-(trifluoromethyl) benzene, 9CI M-1-00135

α,α,α-Trifluoro-p-xylene, 8CI. 4-Methylbenzotrifluoride

[6140-17-6]



$C_8H_7F_3$ M 160.1
Liq. d 1.14. Bp 129°. n_D^{20} 1.4260.

Brownlee, R.T.C. *et al*, *Aust. J. Chem.*, 1980, **33**, 2555 (*F-19 nmr*)
Bromilow, J. *et al*, *J.O.C.*, 1980, **45**, 2429 (*cmr*)
McNeil, J.G. *et al*, *J. Fluorine Chem.*, 1991, **55**, 225 (*synth*)

Methyl(trifluoromethyl) phosphinous acid M-1-00136

$F_3CPMeOH$

$C_2H_4F_3OP$ M 132.0

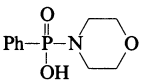
Me ester: [26348-84-5]. *Methyl methyl(trifluoromethyl)phosphinite*
$C_3H_6F_3OP$ M 146.0 Liq. Bp 60.6°.

tert-*Butyl ester:* [26348-85-6]. tert-*Butyl methyl(trifluoromethyl)phosphinite*
$C_6H_{12}F_3OP$ M 188.1 Liq. Bp 113°.

Burg, A.B. *et al*, *J.A.C.S.*, 1970, **92**, 1901 (*synth, ir, pmr, F-19 nmr, P-31 nmr*)

(4-Morpholinyl) phenylphosphinic acid, 9CI M-1-00137

Morpholinophenylphosphinic acid, 8CI



$C_{10}H_{14}NO_3P$ M 227.1

Morpholine salt: [31563-05-0].
Solid. Mp 149-152°.

Me ester: [38938-33-9]. *Methyl (4-morpholinyl)phenylphosphinate*
$C_{11}H_{16}NO_3P$ M 241.2 Cryst. (hexane/CCl_4). Mp 73.5-74.5°. $Bp_{0.03}$ 155° (oven).

Ph ester: [57668-14-1]. *Phenyl (4-morpholinyl) phenylphosphinate. Phenyl phenylphosphonomorpholidate*
$C_{16}H_{18}NO_3P$ M 303.2 Cryst. (EtOH). Mp 134-135°.

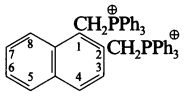
Chloride: [77144-04-8].
$C_{10}H_{13}ClNO_2P$ M 245.6 Cryst. Mp 89-95°.

Gallagher, M.J. *et al*, *J.C.S.(C)*, 1971, 593 (*salt, synth, ir, props*)
Kamai, G.Kh. *et al*, *Zh. Obshch. Khim.*, 1972, **42**, 1295; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1972, **42**, 1290 (*synth, ir*)
Williams, A. *et al*, *J.C.S. Perkin 2*, 1975, 1010 (*Ph ester, synth, uv*)
Felcht, U. *et al*, *Annalen*, 1977, 1309 (*synth, ir, pmr*)

N

[1,2-Naphthalenediylbis (methylene)] bis(triphenylphosphonium)(2+) N-1-00001

1,2-Bis(triphenylphosphonomethyl)naphthalene



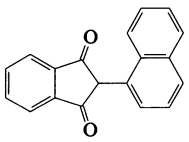
$C_{48}H_{40}P_2^{2\oplus}$ M 678.7 (ion)

Dibromide: [85982-10-1].
$C_{48}H_{40}Br_2P_2$ M 838.5 Cryst. ($MeOH/Et_2O$). Mp 264°, Mp >300°.

Meissner, U.E. *et al*, *Annalen*, 1983, 687 (*synth, ylide*)
Minsky, A., *Synthesis*, 1983, 497 (*synth, use*)

2-(1-Naphthalenyl)-1*H*-indene-1,3(2*H*)-dione, 9CI N-1-00002

2-(1-Naphthyl)-1,3-indanedione. Naphthylin
[1786-03-4]



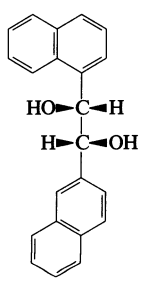
$C_{19}H_{12}O_2$ M 272.3
Anticoagulant. Yellow needles (EtOH). Mp 217-218° (210-211°).

▶ LD_{50} (mus, orl) 900 mg/kg. LD_{50} (mus, ipr) 350 mg/kg. NK6030000.

Dioxime:
$C_{19}H_{14}N_2O_2$ M 302.3 Cryst. Mp 216° dec.

Eckstein, M. *et al*, *CA*, 1959, **53**, 6175 (*synth*)
Shapiro, S.L. *et al*, *J.O.C.*, 1960, **25**, 1860; 1961, **26**, 3580 (*synth, props*)
Perjessy, A. *et al*, *Tetrahedron*, 1971, **27**, 6159 (*ir*)
Fanelli, O., *Arzneim.-Forsch.*, 1975, **25**, 873 (*pharmacol*)
Csoregh, I. *et al*, *Acta Cryst. B*, 1979, **35**, 852 (*cryst struct*)
Murthy, A.R. *et al*, *J. Med. Chem.*, 1985, **28**, 1591 (*synth, props*)

1-(1-Naphthalenyl)-2-(2-naphthalenyl)-1,2-ethanediol, 9CI N-1-00003

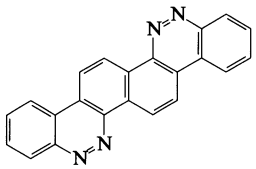


$C_{22}H_{18}O_2$ M 314.3
(1R,2R)-form [159333-30-9]
Cryst. Mp 230°. $[\alpha]_D^{23}$ +130 (c, 1.03 in THF).

Rosini, C. *et al*, *J.O.C.*, 1994, **59**, 7395 (*synth, pmr*)

Naphtho[1,2-*c*:5,6-*c'*] dicinnoline N-1-00004

[157722-29-7]

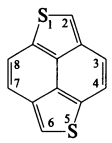


$C_{22}H_{12}N_4$ M 332.3
Greenish-yellow solid. Mp >360°. Subl. >300°.

Shepherd, M.K., *J.C.S. Perkin 1*, 1994, 1055.

Naphtho[1,8-*bc*:5,4-*b',c'*] dithiophene, 9CI N-1-00005

[41879-79-2]

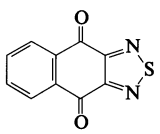


$C_{12}H_6S_2$ M 214.3
Yellow cryst. Mp 93° dec. Air sensitive in soln. and slowly dec. in solid state.

Takimiya, K. *et al*, *Chem. Comm.*, 1994, 1859 (*synth, pmr, cmr, uv*)

Naphtho[2,3-*c*][1,2,5] thiadiazole-4,9-dione, 9CI N-1-00006

[1455-26-1]



$C_{10}H_4N_2O_2S$ M 216.2
Yellow solid. Mp 245-246°.

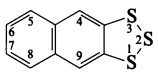
Dioxime:
$C_{10}H_6N_4O_2S$ M 246.2 Yellow needles (dioxan). Mp 270°. Subl. >160°.

Monohydrazone:
$C_{10}H_6N_4OS$ M 230.2 Brown needles (EtOH aq.). Mp 210° dec. Subl. >170°.

Mono-4-methylbenzenesulfonylhydrazone:
Yellowish needles. Mp 229°.

Neeff, R. *et al*, *Chem. Ber.*, 1957, **90**, 1137 (*synth*)
Neidlein, R. *et al*, *Chem. Ber.*, 1982, **115**, 2898 (*deriv, synth, ir, uv, pmr, ms*)
Shi, S. *et al*, *J.O.C.*, 1995, **60**, 1285 (*synth, pmr, cmr, ir, ms*)

Naphtho[2,3-*d*]-1,2,3-trithiole, 9CI N-1-00007



$C_{10}H_6S_3$ M 222.3

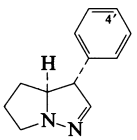
1-Oxide: [146954-01-0].
$C_{10}H_6OS_3$ M 238.3 Yellow cryst. ($CHCl_3$/hexane). Mp 132° dec.

2-Oxide: [146953-92-6].
$C_{10}H_6OS_3$ M 238.3 Yellow plates ($CHCl_3$/hexane). Mp 192° dec.

Yomoji, N. *et al*, *J.C.S. Perkin 1*, 1993, 1995 (*oxide, synth, ir, uv, pmr, cmr, ms*)

Newbouldine† N-1-00008

3a,4,5,6-Tetrahydro-3-phenyl-3H-pyrrolo[1,2-b]pyrazole



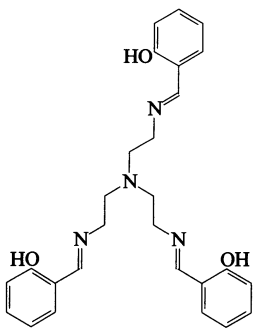
$C_{12}H_{14}N_2$ M 186.2
(±)-form [155416-35-6]
Alkaloid from the root bark of *Newbouldia laevis* (Bignoniaceae). Oil.

4'-Hydroxy: [155416-36-7]. ***4'-Hydroxynewbouldine***
$C_{12}H_{14}N_2O$ M 202.2 Alkaloid from root bark of *N. laevis* (Bignoniaceae). Cryst. (Me_2CO). Mp 155-156°.

Adesanya, S.A. *et al*, *Phytochemistry*, 1994, **35**, 1053 (*isol, uv, ir, pmr, cmr, ms, struct*)

2,2',2''-Nitrilotris(ethane-2,1-diylnitrilomethylidyne) trisphenol N-1-00009

Saltren. Trensal



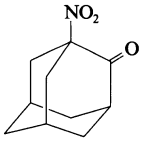
$C_{27}H_{30}N_4O_3$ M 458.5
Obt. by condensation of Tris(2-aminoethyl) amine, T-0-06576 with 2-Hydroxybenzaldehyde, H-0-01667. Trianionic ligand.

Gündüz, N. *et al*, *J.C.S. Perkin 2*, 1985, 899 (*synth*)

1-Nitro-2-adamantanone N-1-00010

1-Nitrotricyclo[3.3.1.1^{3,7}]decanone, 9CI

[162710-73-8]



$C_{10}H_{13}NO_3$ M 195.2
Cryst. solid (CH_2Cl_2/hexane). Mp 170-171°.

Dave, P.R. *et al, J.O.C.*, 1995, **60**, 1895 (*synth, ir, pmr, cmr*)

4-Nitro-1,2-benzenedicarboxaldehyde N-1-00011

4-Nitrophthalaldehyde, 8CI

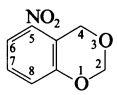
[13209-35-3]

$C_8H_5NO_4$ M 179.1
Needles. Mp 73°. $Bp_{0.5}$ 145-150°.

Kerfanto, M. *et al, Bull. Soc. Chim. Fr.*, 1966, 2966 (*synth*)
Farooq, O., *Synthesis*, 1994, 1035 (*synth, pmr*)

5-Nitro-4*H*-1,3-benzodioxin, 9CI N-1-00012

[50603-42-4]



$C_8H_7NO_4$ M 181.1
Cryst. (EtOH). Mp 75°.

Buehler, C.A. *et al, J.O.C.*, 1941, **6**, 216 (*synth*)
Ando, M. *et al, Bull. Chem. Soc. Jpn.*, 1973, **46**, 2903 (*synth*)
Bowie, J.H. *et al, J.C.S. Perkin 2*, 1975, 724 (*ms*)

7-Nitro-4*H*-1,3-benzodioxin N-1-00013

[50603-43-5]

$C_8H_7NO_4$ M 181.1
Long glistening needles (H_2O). Mp 90.5°.

Buehler, C.A. *et al, J.O.C.*, 1941, **6**, 216 (*synth*)
Ando, M. *et al, Bull. Chem. Soc. Jpn.*, 1973, **46**, 2903 (*synth*)
Bowie, J.H. *et al, J.C.S. Perkin 2*, 1975, 724 (*ms*)

8-Nitro-4*H*-1,3-benzodioxin N-1-00014

[57356-29-3]

$C_8H_7NO_4$ M 181.1
Pale yellow needles (EtOH). Mp 115-116°.

Bowie, J.H. *et al, J.C.S. Perkin 2*, 1975, 724 (*synth, ms*)

1-Nitro-1,3,5-cycloheptatriene, 9CI N-1-00015

[156545-33-4]

$C_7H_7NO_2$ M 137.1
Bright yellow oil with odour similar to nitrobenzene. Mp 3-5°.

▶ Can dec. explosively if stored at r.t.

Burnett, I.J. *et al, Chem. Comm.*, 1994, 1187 (*synth, pmr, cmr*)

2-Nitro-1,3-diphenyl-1-propene N-1-00016

1,1′-(2-Nitro-1-propene-1,3-diyl)bisbenzene, 9CI

[58497-32-8]

$PhCH_2C(NO_2)=CHPh$

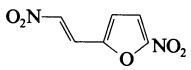
$C_{15}H_{13}NO_2$ M 239.2
Pale yellow cryst. Mp 55-56° (52°).

Yamamura, K. *et al, Bull. Chem. Soc. Jpn.*, 1975, **48**, 3757 (*synth, ir, pmr*)
Kochany, J. *et al, Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1976, **24**, 929 (*synth, ir, pmr*)

Nitrofurilen N-1-00017

2-Nitro-5-(2-nitroethenyl)furan, 9CI. 2-Nitro-5-(2-nitrovinyl)furan, 8CI. 1-Nitro-2-(5-nitro-2-furanyl)ethylene

[830-07-9]



$C_6H_4N_2O_5$ M 184.1
Shows fungicidal and herbicidal activity.

(E)-form [32782-46-0]
Cryst. (EtOH). Mp 137-138°.

Clitheroe, A. *et al, J. Pharm. Pharmacol.*, 1965, **17**, 167 (*activity*)
Kovac, J. *et al, Coll. Czech. Chem. Comm.*, 1977, **42**, 1880 (*synth*)
Kada, R. *et al, Coll. Czech. Chem. Comm.*, 1984, **49**, 2496 (*synth, bibl, pmr, uv*)

6-Nitrohexanoic acid, 9CI N-1-00018

[10269-96-2]

$O_2N(CH_2)_5COOH$

$C_6H_{11}NO_4$ M 161.1
Pale straw-coloured liq. d 1.19. Mp 21-22°. $Bp_{0.3}$ 136°. n_D^{20} 1.4590.

Me ester: [13154-40-0].
$C_7H_{13}NO_4$ M 175.1 Liq. Bp_1 196°.

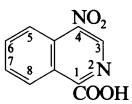
Amide: [22543-31-3].
$C_6H_{12}N_2O_3$ M 160.1 Cryst. (dioxan). Mp 112°.

[13395-05-6]

Matlock, A.S. *et al, J.O.C.*, 1967, **32**, 1995 (*synth, ir, pmr*)
Bischoff, C. *et al, J. Prakt. Chem.*, 1972, **314**, 891 (*amide*)
Ballini, R. *et al, Synth. Commun.*, 1986, **16**, 1781 (*synth, ir, pmr*)

4-Nitro-1-isoquinolinecarboxylic acid, 9CI N-1-00019

[146762-60-9]



$C_{10}H_6N_2O_4$ M 218.1
Cryst. (C_6H_6/hexane). Mp 250-252°.

Nitrile: [146762-59-6]. *1-Cyano-4-nitroisoquinoline*
$C_{10}H_5N_3O_2$ M 199.1 Cryst. (hexane/C_6H_6). Mp 138-140°.

Sugiura, M. *et al, Chem. Pharm. Bull.*, 1992, **40**, 2262 (*synth, ir, pmr*)

5-Nitro-1-isoquinolinecarboxylic acid, 9CI N-1-00020

[75795-40-3]

$C_{10}H_6N_2O_4$ M 218.1
Light yellow cryst. Mp 168-169°.

Me ester: [75795-41-4].
$C_{11}H_8N_2O_4$ M 232.1 Light yellow needles (EtOAc). Mp 162-163°.

Nitrile:
$C_{10}H_5N_3O_2$ M 199.1 Cryst. (EtOH). Mp 198.5-199°.

[77628-99-0]

Kirby, G.W. *et al, J.C.S. Perkin 1*, 1979, 270 (*synth, ir, pmr, nitrile*)
Nishimura, S. *et al, Chem. Pharm. Bull.*, 1980, **28**, 1695 (*synth, ir*)

5-Nitro-3-isoquinolinecarboxylic acid, 9CI 9CI N-1-00021

[80066-72-4]

$C_{10}H_6N_2O_4$ M 218.1
Mp 260-263° dec. Evolves CO_2 above the Mp giving 5-nitroisoquinoline.

Elderfield, R.C. *et al, J.O.C.*, 1958, **23**, 435 (*synth*)

8-Nitro-3-isoquinolinecarboxylic acid N-1-00022

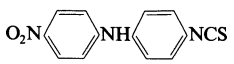
$C_{10}H_6N_2O_4$ M 218.1
Mp 230-240°. Evolves CO_2 above the Mp giving 8-nitroisoquinoline.

Popp, F.D. *et al, J.O.C.*, 1961, **26**, 956 (*synth*)

4-Nitro-4′-isothiocyanatodiphenylamine N-1-00023

4-Isothiocyanato-N-(4-nitrophenyl) benzenamine, 9CI. p-(p-*Nitroanilino)phenyl isothiocyanate, 8CI.* ***Amoscanate, INN.*** *Nithiocyamine. CGP 4540. Go 9333*

[26328-53-0]



$C_{13}H_9N_3O_2S$ M 271.2
Anthelmintic. Mp 204-206°. Relat. to Nitroscanate, N-0-01677.

▶ Exp. retinotoxic. NX9106000.

Ger. Pat., 1 935 338, (1970) (*Agripat*); *CA*, **73**, 25110f (*synth, pharmacol*)
Striebel, H.P., *Experientia*, 1976, **32**, 457 (*pharmacol*)
Vaidaya, A.B. *et al, Br. J. Clin. Pharmacol.*, 1977, **4**, 463 (*tox*)
Rajappa, S. *et al, J.C.S. Perkin 1*, 1979, 2027 (*synth*)
Hardgrove, G.L. *et al, Acta Cryst. C*, 1983, **39**, 616 (*cryst struct*)
Maertins, T. *et al, Arch. Toxicol.*, 1993, **67**, 120 (*tox*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 39.

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, AOA050.

4-Nitro-4*H*-isoxazol-5-one N-1-00024

4-Nitro-3-isoxazolin-5-one

$C_3H_2N_2O_4$ M 130.0

Pyridinium salt: Pale yellow needles. Mp 141-142° dec. Exists in *aci*-nitro form.

Nishiwaki, N. *et al*, *J. Het. Chem.*, 1995, **32**, 473 (*synth*, *pmr*)

6-Nitro-2,3-naphthalenedicarboxylic acid N-1-00025

[139451-35-7]

$C_{12}H_7NO_6$ M 261.1

No phys. props. reported.

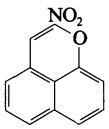
Di-Et ester: [155534-58-0].
$C_{16}H_{15}NO_6$ M 317.2 Mp 139-141°.

Makosza, M. *et al*, *Synthesis*, 1994, 264 (*di-Et ester*, *synth*)

2-Nitronaphtho[1,8-*bc*]pyran, 9CI N-1-00026

2-Nitro-1-oxaphenalene

[105052-38-8]



$C_{12}H_7NO_3$ M 213.1

Compd. and its subst. derivs. are used in mutagenicity studies. Brick-red cryst. (EtOH). Mp 117°.

▶ Highly genotoxic, prob. carcinogen.

Royer, R. *et al*, *Eur. J. Med. Chem.* (*Chim. Ther.*), 1986, **21**, 352 (*synth*)

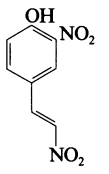
Buisson, J.-P. *et al*, *J. Het. Chem.*, 1988, **25**, 539 (*synth*)

Salmon, R.J. *et al*, *Carcinogenesis* (*London*), 1989, **10**, 803 (*tox*)

2-Nitro-4-(2-nitroethenyl)phenol, 9CI N-1-00027

2-Nitro-4-(2-nitrovinyl)phenol

[2084-92-6]



$C_8H_6N_2O_5$ M 210.1

Isol. from the leaves of *Sonneratia acida*. Yellow needles (AcOH/MeOH). Mp 152° (synthetic).

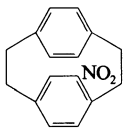
Japan. Pat., 64 26 960, (1964); *CA*, **62**, 14569e (*synth*)

Bose, A.K. *et al*, *Oceanogr. Indian Ocean*, 1992, 407; *CA*, **120**, 212589 (*isol*, *struct*)

4-Nitro[2.2]paracyclophane N-1-00028

5-Nitrotricyclo[8.2.2.2^{4,7}]hexadeca-4,6,10,12,13,15-hexaene, *9CI*

[10122-96-0]



$C_{16}H_{15}NO_2$ M 253.3

(±)-*form*

Light yellow needles (EtOH). Mp 155.5-156.5°.

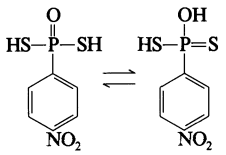
Cram, D.J. *et al*, *J.A.C.S.*, 1955, **77**, 6289 (*synth*)

Norcross, B.E. *et al*, *J.O.C.*, 1967, **32**, 220 (*synth*, *ir*)

Ernst, L., *Annalen*, 1995, 13 (*pmr*, *cmr*, *conformn*)

(4-Nitrophenyl)phosphonodithoic acid, 9CI N-1-00029

4-Nitrophenyldithiophosphonic acid



$C_6H_6NO_3PS_2$ M 235.2

Tautomeric.

Phosphoryl-form

S,S-*Di-Me ester:* [30381-63-6]. S,S-*Dimethyl (4-nitrophenyl)phosphonodithioate*
$C_8H_{10}NO_3PS_2$ M 263.2 Solid. Mp 81.5-83°.

S,S-*Di-Et ester:* [30381-64-7]. S,S-*Diethyl (4-nitrophenyl)phosphonodithioate*
$C_{10}H_{14}NO_3PS_2$ M 291.3 Liq. $Bp_{0.01}$ 175-180°.

S,S-*Dipropyl ester:* [30381-65-8]. S,S-*Dipropyl (4-nitrophenyl)phosphonodithioate*
$C_{12}H_{18}NO_3PS_2$ M 319.3 Liq. $Bp_{0.01}$ 185-187°.

Płazek, E. *et al*, *Rocz. Chem.*, 1970, **44**, 681 (*synth*, *ir*)

1-Nitro-2-phenylpropane N-1-00030

(*1-Methyl-2-nitroethyl)benzene*. *β-Nitrocumene*

[7796-75-0]

$H_3CCHPhCH_2NO_2$

$C_9H_{11}NO_2$ M 165.1

(±)-*form*

Oil.

Abbenante, G. *et al*, *Aust. J. Chem.*, 1994, **47**, 1441 (*synth*)

3-Nitro-2-phenyl-1-propylamine N-1-00031

β-(Nitromethyl)benzeneethanamine, *9CI*

[159112-20-6]

$O_2NCH_2CHPhCH_2NH_2$

$C_9H_{12}N_2O_2$ M 180.2

(±)-*form*

Needles (as hydrochloride). Mp 205-206° (hydrochloride).

Abbenante, G. *et al*, *Aust. J. Chem.*, 1994, **47**, 1441 (*synth*)

(1-Nitropropyl)phosphonic acid N-1-00032

$H_3CCH_2CH(NO_2)P(O)(OH)_2$

$C_3H_8NO_5P$ M 169.0

Di-Me ester: [60593-27-3]. *Dimethyl (1-nitropropyl)phosphonate*
$C_5H_{12}NO_5P$ M 197.1 Liq. Bp_2 103°. pK_a 6.74 (50% EtOH). n_D^{20} 1.4442.

Di-Et ester: [136496-87-2]. *Diethyl (1-nitropropyl)phosphonate*
$C_7H_{16}NO_5P$ M 225.1 Liq. Bp_3 130°. n_D^{20} 1.4411.

Diisopropyl ester: Diisopropyl (1-nitropropyl) phosphonate
$C_9H_{20}NO_5P$ M 253.2 Liq. Bp_1 98-101°. n_D^{20} 1.4342.

Petrov, K.A. *et al*, *Zh. Obshch. Khim.*, 1976, **46**, 1250; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1976, **46**, 1230.

Petrov, K.A. *et al*, *Zh. Obshch. Khim.*, 1979, **49**, 90; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1979, **49**, 75 (*Di-Me ester*)

Zoń, J., *Synthesis*, 1984, 661.

(3-Nitropropyl)phosphonic acid N-1-00033

$O_2NCH_2CH_2CH_2P(O)(OH)_2$

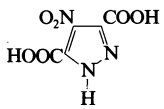
$C_3H_8NO_5P$ M 169.0

Di-Et ester: [33475-85-3]. *Diethyl (3-nitropropyl)phosphonate*
$C_7H_{16}NO_5P$ M 225.1 Liq. d_4^{20} 1.17. $Bp_{0.1}$ 111-112°. n_D^{20} 1.4421.

Mastryukova, T.A. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1971, 1353; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1971, 1264.

4-Nitro-1*H*-pyrazole-3,5-dicarboxylic acid, 9CI N-1-00034

[62078-43-7]



$C_5H_3N_3O_6$ M 201.0

Solid. Mp 206°.

Di-Me ester: [59694-23-4].
$C_7H_7N_3O_6$ M 229.1 Solid (H_2O). Mp 122-124°.

Dihydrazide: [62063-00-7].
$C_5H_7N_7O_4$ M 229.1 Cryst. (EtOH aq.). Mp 178°.

1-Me, di-Me ester: [159427-78-8].
$C_8H_9N_3O_6$ M 243.1 Solid (EtOAc/petrol). Mp 135°.

[162937-26-0]

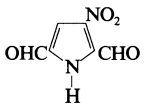
Latypov, N.V. *et al*, *Khim. Geterotsikl. Soedin.*, 1976, **12**, 1649; *J. Het. Chem. USSR*, 1976, **12**, 1355 (*di-Me ester*, *dihydrazide*, *synth*, *ir*)

Baraldi, P.G. *et al*, *J. Med. Chem.*, 1994, **37**, 4329 (*synth*)

3-Nitro-1*H*-pyrrole-2,5-dicarboxaldehyde, 9CI N-1-00035

2,5-Diformyl-3-nitropyrrole

[153850-78-3]



$C_6H_4N_2O_4$ M 168.1

Cryst. (Me_2CO/pentane). Mp 140-141°.

Cadamuro, S. *et al*, *J.C.S. Perkin 1*, 1993, 2939 (*synth, ir, pmr, cmr*)

1-Nitropyrrolidine, 9CI N-1-00036

[3760-55-2]

$C_4H_8N_2O_2$ M 116.1

Cryst. (petrol). Mp 55-57° (49-51°).

Bottaro, J.C. *et al*, *J.O.C.*, 1987, **52**, 2292 (*synth*)

Suri, S.C. *et al*, *Synthesis*, 1988, 743 (*synth, ir, pmr, cmr*)

Shishkov, I.F. *et al*, *Zh. Strukt. Khim.*, 1992, **33**, 46; *CA*, **117**, 76981a (*struct*)

Daszikiewicz, Z. *et al*, *Org. Prep. Proced. Int.*, 1994, **26**, 337 (*synth*)

3-Nitrosobiphenyl N-1-00037

[105361-86-2]

$C_{12}H_9NO$ M 183.2

Ioannides, C. *et al*, *Carcinogenesis* (*London*), 1989, **10**, 1403; *CA*, **111**, 128739a (*synth*)

4-Nitrosobiphenyl N-1-00038

[10125-76-5]

$C_{12}H_9NO$ M 183.2

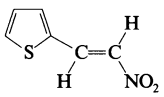
Yellow solid. Mp 74-75°.

Brill, E., *Experientia*, 1974, **30**, 835 (*synth*)

2-(2-Nitrovinyl)thiophene, 8CI N-1-00039

2-(2-Nitroethenyl)thiophene, 9CI. 1-Nitro-2-(2-thienyl)ethylene

[874-84-0]



$C_6H_5NO_2S$ M 155.1

(E)-form [34312-77-1]

Yellow. Mp 80°.

Dressler, M.L. *et al*, *J. Het. Chem.*, 1970, **7**, 1257 (*synth*)

Satonaka, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1985, **58**, 3651 (*pmr, cmr*)

Bourguignon, J. *et al*, *Can. J. Chem.*, 1985, **63**, 2354 (*synth*)

1,20-Nonacosadiene N-1-00040

[28914-19-4]

$H_3C(CH_2)_7CH{=}CH(CH_2)_{17}CH{=}CH_2$

$C_{29}H_{56}$ M 404.7

(E)-form [104899-46-9]

Isol. from the alga *Botryococcus braunii*.

(Z)-form [104899-41-4]

Isol. from *B. braunii*.

Metzger, P. *et al*, *Phytochemistry*, 1986, **25**, 1869; 1993, **33**, 1125 (*isol, pmr, cmr*)

1,19-Nonadecanediol N-1-00041

[7268-65-7]

$HOCH_2(CH_2)_{17}CH_2OH$

$C_{19}H_{40}O_2$ M 300.5

Leaflets (C_6H_6). Mp 101° (95-96°).

Chuit, P. *et al*, *Helv. Chim. Acta*, 1929, **12**, 850 (*synth*)

Lukeš, R. *et al*, *Chem. Listy*, 1958, **52**, 1926; *CA*, **53**, 3055g (*synth*)

Percec, V. *et al*, *Macromolecules*, 1990, **23**, 3509 (*synth, pmr*)

3,7-Nonadiyn-1-ol N-1-00042

[160109-63-7]

$H_3CC{\equiv}CCH_2CH_2C{\equiv}CCH_2CH_2OH$

$C_9H_{12}O$ M 136.1

No phys. props. descr.

Bao, J. *et al*, *J.A.C.S.*, 1994, **116**, 7616 (*synth, ir, pmr, cmr, ms*)

1,1,2,2,3,3,4,4,4-Nonafluoro-1-butanesulfonic acid, 9CI N-1-00043

Perfluorobutyric acid

[375-73-5]

$F_3CCF_2CF_2CF_2SO_3H$

$C_4HF_9O_3S$ M 300.1

One of the strongest known acids, with synthetic applications. Liq. Bp 210-212°, Bp_{15} 120-130°.

Ag salt: [116831-41-5].
Mp >250°.

Me ester: [6401-03-2].
$C_5H_3F_9O_3S$ M 314.1 Liq. Mp −13.5°. Bp 155.1°, Bp_{40} 75°.

Trifluoromethyl ester: [79410-57-4].
$C_5F_{12}O_3S$ M 368.1 Liq. Mp −78.9°. Bp 93.6°.

Ph ester: [25628-11-9].
$C_{10}H_5F_9O_3S$ M 376.1 Liq. Bp_{15} 100-101°, Bp_{12} 99°.

Anhydride: [36913-91-4].
$C_8F_{18}O_5S_2$ M 582.1 Liq. Bp_{14} 84°.

Gramstad, J. *et al*, *J.C.S.*, 1957, 2640; 1956, 173 (*synth*)

Subramanian, L.R. *et al*, *Chem. Ber.*, 1972, **105**, 1465 (*anhydride*)

Brunel, D. *et al*, *Bull. Soc. Chim. Fr.*, 1979, 249 (*use*)

John, K.K. *et al*, *J.O.C.*, 1981, **46**, 5081 (*deriv*)

Subramanian, L.R. *et al*, *Synthesis*, 1984, 481 (*synth, ir, pmr, deriv*)

Frasch, M. *et al*, *Chem. Ber.*, 1991, **124**, 1805 (*synth, ester*)

Conte, L. *et al*, *J. Fluorine Chem.*, 1991, **53**, 277 (*synth, ir, pmr, deriv*)

3,3,4,4,5,5,6,6,6-Nonafluoro-1-hexene, 9CI, 8CI N-1-00044

[19430-93-4]

$F_3C(CF_2)_3CH{=}CH_2$

$C_6H_3F_9$ M 246.0

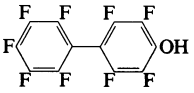
Bp 59-59.5°.

Kim, Y.K. *et al*, *J.O.C.*, 1973, **38**, 1615.

2,2′,3,3′,4,5,5′,6,6′-Nonafluoro-4′-hydroxybiphenyl N-1-00045

2,2′,3,3′,4′,5,5′,6,6′-Nonafluoro-[1,1′-biphenyl]-4-ol, 9CI. Perfluoro-4-biphenylol. 2,3,5,6-Tetrafluoro-4-(pentafluorophenyl)phenol

[2894-87-3]



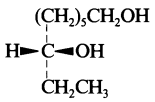
$C_{12}HF_9O$ M 332.1

Cryst. Mp 119-120°.

Buxton, M.W. *et al*, *J. Fluorine Chem.*, 1973, **2**, 231 (*synth*)

1,7-Nonanediol N-1-00046

[4469-84-5]



(*R*)-*form*

$C_9H_{20}O_2$ M 160.2

(R)-form [161513-89-9]

Liq. Bp_1 138°. $[\alpha]_D^{25}$ −9.5 (c, 1.8 in $CHCl_3$).

(±)-form

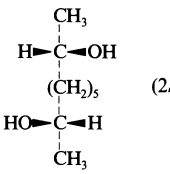
Liq. Bp_2 134-135°.

Cekovic, Z. *et al*, *Croat. Chem. Acta*, 1985, **58**, 671 (*synth, ir, pmr*)

Paolucci, C. *et al*, *J.O.C.*, 1995, **60**, 169 (*synth*)

2,8-Nonanediol, 9CI, 8CI N-1-00047

[39997-24-5]



(2*S*,8*S*)-*form*

$C_9H_{20}O_2$ M 160.2

Liq.

(2S,8S)-form [141667-22-3]

Liq. $[\alpha]_D^{23}$ +14.48 (c, 2.63 in $CHCl_3$) (>99% ee).

Keinan, E. *et al*, *J.O.C.*, 1992, **57**, 3631 (*synth, pmr, cmr, ir*)

Sinha, S.C. *et al*, *J.O.C.*, 1993, **58**, 7789 (*synth*)

8-Nonene-2,5-dione, 9CI N-1-00048

[5312-86-7]

$H_2C{=}CHCH_2CH_2COCH_2CH_2COCH_3$

$C_9H_{14}O_2$ M 154.2

Liq. Bp_8 180°.

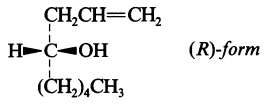
Betancourt de Perez, R.M. *et al*, *J.O.C.*, 1986, **51**, 2039 (*synth*)

Pecunioso, A. *et al*, *J.O.C.*, 1989, **54**, 2391 (*pmr, cmr, ms*)

Ballini, R., *Synthesis*, 1993, 687 (*synth, pmr*)

1-Nonen-4-ol, 9CI N-1-00049

[35192-73-5]



(*R*)-form

$C_9H_{18}O$ M 142.2

(R)-form [91525-93-8]
$[\alpha]_D^{23}$ +4.0 (c, 2 in $CHCl_3$).

(±)-form [106756-94-9]
Liq. Bp_{13} 105-110°. n_D^{20} 1.4406.

Me ether: [106650-76-4]. *4-Methoxy-1-nonene, 9CI*
$C_{10}H_{20}O$ M 156.2 Liq. Bp_2 57-59°.

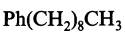
[90246-13-2]

Schlosser, M. *et al*, *Tetrahedron*, 1990, **46**, 2411 (*Me ether, synth*)
Sato, F. *et al*, *Tet. Lett.*, 1991, **32**, 371 (*R-form, pmr, cmr*)
Imai, T. *et al*, *Synthesis*, 1993, 395 (*synth*)

Nonylbenzene, 9CI N-1-00050

1-Phenylnonane, 8CI

[1081-77-2]



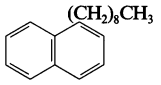
$C_{15}H_{24}$ M 204.3
Liq. Fp −24°. Bp 282.0°.

Adv. Chem. Ser., 1955, **15**, 104 (***props***)
Minisci, F. *et al*, *Tetrahedron*, 1972, **28**, 2415 (*ms*)
Castle, P.L. *et al*, *Tet. Lett.*, 1986, **27**, 6013 (*synth*)
Cahiez, G. *et al*, *Synlett*, 1993, 45 (*synth*)

1-Nonylnaphthalene N-1-00051

1-(1-Naphthalenyl)nonane

[26438-26-6]



$C_{19}H_{26}$ M 254.4
d^{20} 0.937. Fp 8°. Bp 372°, Bp_1 157°. n_D^{20} 1.5477.

Adv. Chem. Ser., 1955, **15**, 230 (***props***)

2-Nonylnaphthalene N-1-00052

1-(2-Naphthalenyl)nonane

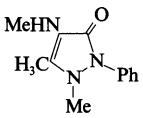
$C_{19}H_{26}$ M 254.4
d^{20} 0.930. Fp 12°. Bp 372°, Bp_1 157°. n_D^{20} 1.5454.

Adv. Chem. Ser., 1955, **15**, 231 (***props***)

Noramidopyrine N-1-00053

1,2-Dihydro-1,5-dimethyl-4-(methylamino)-2-phenyl-3H-pyrazol-3-one, 9CI. 4-(Methylamino)antipyrine, 8CI. Calmagine

[519-98-2]



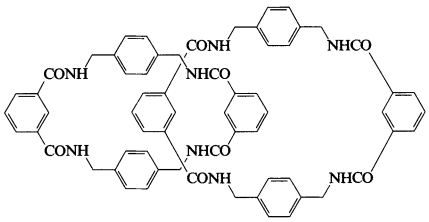
$C_{12}H_{15}N_3O$ M 217.2
Metab. of Dipyrone, D-0-12710 and Aminophenazone, A-0-03375. Active subst. in many drugs having antipyretic and analgesic effects. Cryst. (Et_2O/petrol). Mp 58-60°.

▶ LD_{50} (rat, ipr) 1288 mg/kg. CD2995850.

Chiti, W., *Farmaco, Ed. Sci.*, 1960, **15**, 679; *CA*, **57**, 16597c (*synth*)
Banci, F. *et al*, *Arzneim.-Forsch.*, 1971, **21**, 1665 (*pharmacol*)
Noda, A. *et al*, *Chem. Pharm. Bull.*, 1976, **24**, 3229 (*metab*)
Lissel, M. *et al*, *J. Chem. Res., Synop.*, 1989, 312 (*synth, ir, pmr*)

O

Octaamide[2]catenane O-1-00001



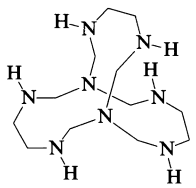
$C_{64}H_{56}N_8O_8$ M 1065.1
Readily obt. in 1-step octamerisation. Smallest catenane so far obt. Mp 315° dec.

Johnston, A.G. *et al*, *Angew. Chem., Int. Ed.*, 1995, **34**, 1209 (*synth, ms, pmr, cmr, cryst struct*)

1,3;6,8,10,13,16,19-Octaazabicyclo[6.6.6]eicosane, 9CI O-1-00002

Sepulchrate

[63413-08-1]



$C_{12}H_{30}N_8$ M 286.4
Characterised as metal complexes. Macrobicyclic nitrogen cage for metal ions.

[62994-31-4, 75592-24-4, 148949-71-7, 148977-71-3]

Creaser, I.I. *et al*, *J.A.C.S.*, 1977, **99**, 3181; 1982, **104**, 6016 (*synth, cryst struct, complex*)
Dubiciki, L. *et al*, *J. Phys. Chem.*, 1984, **88**, 4254 (*cd, Raman, Co complex*)
Bacchi, A. *et al*, *Acta Cryst. C*, 1993, **49**, 1163 (*cryst struct, complex*)

10-Octacosanone O-1-00003

[31617-35-3]

$H_3C(CH_2)_{17}CO(CH_2)_8CH_3$

$C_{28}H_{56}O$ M 408.7
Constit. of the seeds of *Achyranthes aspera*.

Baser, I.A., *CA*, 1971, **74**, 99408 (*synth*)
Ali, M., *Orient. J. Chem.*, 1993, **9**, 84 (*isol*)

9,12,17-Octadecatrienoic acid O-1-00004

$H_2C{=}CH(CH_2)_3CH{=}CHCH_2CH{=}CH(CH_2)_7COOH$

$C_{18}H_{30}O_2$ M 278.4
(9Z,12Z)-form [139959-66-3]
Isol. from the phospholipids of the pea aphid *Acyrthosiphon pisum*.

Febvay, G. *et al*, *Experientia*, 1993, **49**, 915 (*isol*)

Octadecylphosphonic acid O-1-00005

1-Phosphonooctadecane. 1-Octadecanephosphonic acid

[4724-47-4]

$H_3C(CH_2)_{17}P(O)(OH)_2$

$C_{18}H_{39}O_3P$ M 334.4
Solid. Mp 98.5-99°.

Dibutyl ester: Dibutyl octadecylphosphonate $C_{26}H_{55}O_3P$ M 446.6 Liq. d_4^{25} 0.90. Bp_2 248-250°. n_D^{25} 1.4499.

Kosolapoff, G.M., *J.A.C.S.*, 1945, **67**, 1180.

1,3-Octadiene, 9CI O-1-00006

[1002-33-1]

$H_3C(CH_2)_3CH{=}CHCH{=}CH_2$

C_8H_{14} M 110.1
(E)-form [39491-65-1]
Liq. Bp 123-126°. n_D^{21} 1.4483. Obt. mixed with *ca.* 30% *Z* isomer.

Prévost, C. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 2485 (*synth*)
Beger, J. *et al*, *J. Prakt. Chem.*, 1984, **326**, 12 (*synth, pmr, ms*)
Kitahara, T. *et al*, *Synthesis*, 1994, 692 (*synth, ir, pmr*)

1,1,1,3,3,4,4,4-Octafluoro-2-butanone, 9CI O-1-00007

Perfluorobutanone

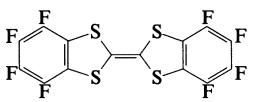
[337-20-2]

$F_3CCF_2COCF_3$

C_4F_8O M 216.0
Liq. Ir ν(CO) 1800 cm^{-1}. Hygroscopic.

Holub, F.F. *et al*, *J.A.C.S.*, 1950, **72**, 4879 (*synth*)
Delfino, J.J. *et al*, *Inorg. Chem.*, 1966, **5**, 308 (*synth, ir*)
Husain, S.Z. *et al*, *Bull. Soc. Chim. Fr.*, 1986, 891 (*synth, ir*)

Octafluorodibenzotetrathiafulvalene O-1-00008



$C_{14}F_8S_4$ M 448.4
Dark red solid. Mp 175-177°.

Purrington, S.T. *et al*, *Synthesis*, 1994, 460 (*synth, cmr, F-19 nmr, ir, uv, ms, cryst struct*)

1,1,2,2,3,3,4,4-Octafluoro-1,4-diiodobutane O-1-00009

1,4-Diiodoperfluorobutane

[375-50-8]

$ICF_2CF_2CF_2CF_2I$

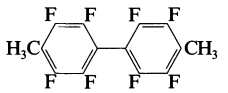
$C_4F_8I_2$ M 453.8
Patented for use as hydraulic fluid and in preparation of special rubbers. d 2.48. Mp −9°. Bp_{100} 85°. n_D^{20} 1.4300.

Haszeldine, R.N., *J.C.S.*, 1953, 1764 (*uv*)
Hauptschein, M. *et al*, *J.O.C.*, 1953, **18**, 235 (*synth*)

2,2′,3,3′,5,5′,6,6′-Octafluoro-4,4′-dimethylbiphenyl, 9CI O-1-00010

*2,2′,3,3′,5,5′,6,6′-Octafluoro-*p,p′*-bitolyl, 8CI. 4,4′-Dimethyloctafluorobiphenyl*

[26475-18-3]



$C_{14}H_6F_8$ M 326.1
Mp 148-149°.

Respess, W.L. *et al*, *J. Organomet. Chem.*, 1970, **22**, 251.
Kobrina, L.S. *et al*, *Zh. Org. Khim.*, 1977, **13**, 1246; *J. Org. Chem. USSR (Engl. Transl.)*, 1977, **13**, 1145 (*synth, F-19 nmr, ir, uv*)

2,2,3,3,4,4,5,5-Octafluoro-1,6-hexanediol O-1-00011

Perfluoro-1,6-hexanediol

[355-74-8]

$HOCH_2CF_2CF_2CF_2CF_2CH_2OH$

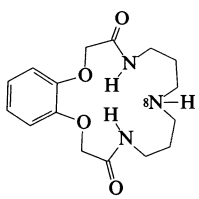
$C_6H_6F_8O_2$ M 262.0
Tan solid. Mp 67-70°. Bp_3 100°.

Bis(4-methylbenzenesulfonyl): [58191-47-2]. Solid. Mp 134-136°.

McBee, E.T. *et al*, *J.A.C.S.*, 1952, **74**, 444 (*synth*)
Greenwald, R.B. *et al*, *J.O.C.*, 1976, **41**, 1469, 1470 (*synth*)
Mikisheva, L.I. *et al*, *CA*, 1981, **95**, 132219z (*synth*)

5,6,7,8,9,10,11,12-Octahydro-2*H*-1,15,4,8,12-benzodioxatriazacycloheptadecine-3,13(4*H*,14*H*)-dione, 9CI O-1-00012

[134142-96-4]



$C_{16}H_{23}N_3O_4$ M 321.3
Parent compd. and derivs. are efficient cation complexing and extraction agents. Mp 187°.

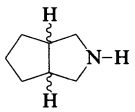
8-Me: [145902-21-2].
$C_{17}H_{25}N_3O_4$ M 335.4 Mp 90°.
8-(2-Cyanoethyl): [145902-25-6].
$C_{19}H_{26}N_4O_4$ M 374.4 Mp 115°.

Kumar, S. *et al, J.C.S. Perkin 1*, 1992, 3049 (*synth, pmr, cmr*)
Hundal, G. *et al, Acta Cryst. C*, 1995, **51**, 1459 (*cryst struct, deriv*)

Octahydrocyclopenta[*c*]pyrrole O-1-00013

3-Azabicyclo[3.3.0]octane

[5661-03-0]



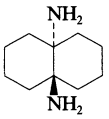
$C_7H_{13}N$ M 111.1
Liq. Bp 158.5°, Bp_{50} 73-75°.
Hydrochloride: Cryst. (EtOH/EtOAc). Mp 134.5-135.5°.
Picrate: Yellow cryst. Mp 147-148°.
Picrolonate: Cryst. (EtOH). Mp 238.5° dec.
N-(*4-Methylbenzenesulfonyl*)*:* [54104-88-0]. Cryst. Mp 45-46°.
N-*Me:* [55100-42-0].
$C_8H_{15}N$ M 125.2 Liq. Bp 152-153°. n_D^{20} 1.4651.
N-*Me, picrate:* [55100-43-1]. Yellow cryst. (EtOH). Mp 203-205°.
N,N-*Di-Me:*
$C_9H_{18}N^{\oplus}$ M 140.2 (ion) Cryst. (as iodide). Mp 197-198° (iodide).

[1468-87-7, 85960-51-6]

Griot, R., *Helv. Chim. Acta*, 1959, **42**, 67 (*synth, deriv*)
Muramaya, K. *et al, Yakugaku Zasshi*, 1965, **85**, 130 (*synth, deriv*)
Khandewal, G.D. *et al, J.C.S. Perkin 1*, 1974, 891 (*N-(4-methylbenzenesulfonyl)*)
Beugelmans, R. *et al, Can. J. Chem.*, 1985, **63**, 725 (*N-Me*)
Roussi, G. *et al, Tetrahedron*, 1991, **47**, 5161 (*synth, pmr*)

Octahydro-4*a*,8*a*-naphthalenediamine O-1-00014

9,10-Decalindiamine. 9,10-Diaminodecalin



(*4aRS,8aRS*)-*form*

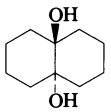
$C_{10}H_{20}N_2$ M 168.2
(4aRS,8aRS)-form
trans-*form*
Mp 70°. Bp_{12} 120° approx.
Picrate (1:2): Needles. Mp 262-264°.
(4aRS,8aSR)-form
cis-*form*
Mp 41°. Bp_{12} 121°.
Picrate (1:1): Mp 236° dec.
Picrate (1:2): Mp 242-247° dec.
Hydrate (1:2): Mp 47°.
N,N′-*Di-Ac:*
$C_{14}H_{24}N_2O_2$ M 252.3 Mp 242°.

Plattner, P.A. *et al, Helv. Chim. Acta*, 1944, **27**, 220.

Octahydro-4*a*,8*a*-naphthalenediol, 9CI O-1-00015

9,10-Decalindiol. Bicyclo[4.4.0]decane-1,6-diol. 9,10-Dihydroxydecalin

[49578-06-5]



$C_{10}H_{18}O_2$ M 170.2
(4aRS,8aRS)-form [57289-63-1]
trans-*form*
Cryst. (petrol). Mp 96°.
Ac:
$C_{12}H_{20}O_3$ M 212.2 Cryst. Mp 168-169°.

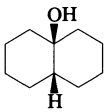
[28795-95-1]

Hückel, W. *et al, Annalen*, 1933, **502**, 99 (*synth*)
Hückel, W. *et al, Chem. Ber.*, 1956, **89**, 2098 (*synth*)

Octahydro-4*a*(2*H*)-naphthalenol, 9CI O-1-00016

Bicyclo[4.4.0]decan-1-ol. 9-Decalol. 9-Hydroxydecalin

[55693-34-0]



(*4aRS,8aRS*)-*form*

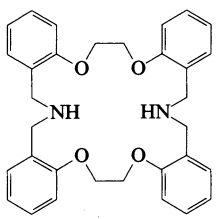
$C_{10}H_{18}O$ M 154.2
(4aRS,8aRS)-form [3574-58-1]
cis-*form*
Cryst. (petrol). Mp 64.5°.
(4aRS,8aSR)-form [1654-87-1]
trans-*form*
Cryst. Mp 50-51°.

[36144-11-3, 99299-13-5]

Durland, J.R. *et al, J.A.C.S.*, 1939, **61**, 429 (*synth*)
Mello, R. *et al, J.A.C.S.*, 1989, **111**, 6749 (*synth, ir, pmr, cmr, ms*)
DesMarteau, D.D. *et al, J.A.C.S.*, 1993, **115**, 4897.

6,7,14,15,21,22,29,30-Octahydro-13*H*,28*H*-tetrabenzo[*e,j,p,u*][1,4,12,15,8,19]tetraoxadiazacyclodocosine, 9CI O-1-00017

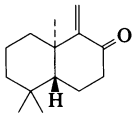
[156339-67-2]



$C_{32}H_{34}N_2O_4$ M 510.6
Cryst. (C_6H_6). Mp 169°.

Atkinson, I.M. *et al, Aust. J. Chem.*, 1994, **47**, 1155 (*synth, pmr, cmr*)

Octahydro-5,5,8*a*-trimethyl-1-methylene-2(1*H*)-naphthalenone, 9CI O-1-00018



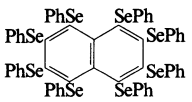
(*4aR,8aR*)-*form*

$C_{14}H_{22}O$ M 206.3
Synthon for triterpene and sesquiterpene natural prods.; intermed. for 8,12-Epoxy-13,14,15,16-tetranorlabdane, E-0-00193.
(4aR,8aR)-form [108944-89-4]
(+)-trans-*form*
Needles (pentane). Mp 55-56°. $[\alpha]_D^{23}$ +71.9 (c, 0.695 in $CHCl_3$).
(4aS,8aS)-form [59633-90-8]
(−)-trans-*form*
Needles (pentane). Mp 55.5-56.5°. $[\alpha]_D^{23}$ −69.6 (c, 0.5 in $CHCl_3$).
(4aRS,8aRS)-form [65556-26-5]
(±)-trans-*form*
Pale yellow oil.
2,4-Dinitrophenylhydrazone: Orange needles ($CHCl_3$/MeOH). Mp 183-184.5°.

Eschenmoser, A. *et al, Helv. Chim. Acta*, 1957, **40**, 1900 (*synth, ir, uv*)
White, J.D. *et al, J.O.C.*, 1985, **50**, 1939 (*synth, pmr*)
Mori, K. *et al, Bull. Soc. Chim. Belg.*, 1986, **95**, 771 (*synth, ir, pmr*)
Marsaioli, A.J. *et al, J.C.S. Perkin 1*, 1989, 559 (*synth, pmr, ms*)
Cortes, M. *et al, Synth. Commun.*, 1989, **19**, 2841 (*synth, pmr*)
Snowden, R.L. *et al, Tet. Lett.*, 1991, **32**, 4119 (*synth, pmr, cmr, ms*)
Nair, M.S. *et al, Synth. Commun.*, 1994, **24**, 1085 (*synth, pmr, cmr, ir*)

Octakis(phenylseleno) naphthalene O-1-00019

[144096-04-8]

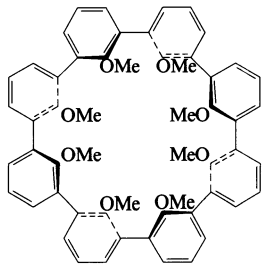


$C_{58}H_{40}Se_8$ M 1368.6

MacNicol, D.D. *et al, Chem. Comm.*, 1985, 1649.
MacNicol, D.D. *et al, Acta Cryst. C*, 1992, **48**, 1557 (*synth, cryst struct*)

41,42,43,44,45,46,47,48-Octamethoxynonacyclo [35.3.1.1^{2,6}.1^{7,11}.1^{12,16}.1^{17,21}.1^{22,26}.1^{27,31}.1^{32,36}]octatetraconta-1(41),2,4,6(48),7,9,11(47),12,14,16(46),17,19,21(45),22,24,26(44),27,29,31(43),32,34,36(42),37,39-tetracosaene, 9CI O-1-00020

[110569-94-3]

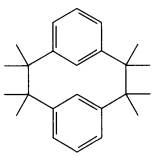


$C_{56}H_{48}O_8$ M 848.9
Cavitand. Cryst. (CH_2Cl_2/Me_2CO). Mp 348-350°.

Cram, D.J. *et al*, *J.A.C.S.*, 1987, **109**, 7068 (*synth, cryst struct, pmr, cmr, ms*)
Trueblood, K.N. *et al*, *Acta Cryst. C*, 1995, **51**, 894 (*cryst struct*)

Octamethyl[2.2]metacyclophane O-1-00021

[93958-99-7]

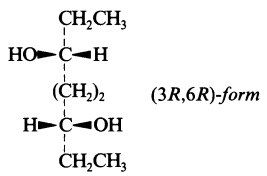


$C_{24}H_{32}$ M 320.5
Powder. Mp 221-224°.

Gajewski, J.J. *et al*, *J.A.C.S.*, 1994, **116**, 5150 (*synth, pmr, cmr*)

3,6-Octanediol O-1-00022

[24434-09-1]



(*3R,6R*)-*form*

$C_8H_{18}O_2$ M 146.2

(3R,6R)-form [129619-37-0]
Cryst. solid (Et_2O). Mp 51-52°. $[\alpha]_D^{25}$ −22.8 (c, 1 in $CHCl_3$) (>99% ee).

(3S,6S)-form [136705-66-3]
$[\alpha]_D^{25}$ +22.8 (c, 1 in $CHCl_3$).

Cyclic sulfate: [136705-67-4]. *4,7-Diethyl-1,3,2-dioxathiepane 2,2-dioxide, 9CI*
$C_8H_{16}O_4S$ M 208.2 Cryst. (Et_2O/hexane). Mp 79.5-80.5°. $[\alpha]_D^{25}$ +28.6 (c, 1 in $CHCl_3$).

[151124-02-6]

Sudweeks, W.H. *et al*, *J.O.C.*, 1975, **40**, 1131 (*synth*)
Burk, M.J. *et al*, *Tetrahedron: Asymmetry*, 1991, **2**, 569 (*synth, pmr, cmr*)
Burk, M.J. *et al*, *J.A.C.S.*, 1993, **115**, 10125 (*sulfate, synth, pmr, cmr*)

Octanethioic acid, 9CI O-1-00023

Thiocaprylic acid

[7530-92-9]

$H_3C(CH_2)_5CH_2C(O)SH \rightleftharpoons H_3C(CH_2)_5CH_2C(S)OH$

$C_8H_{16}OS$ M 160.2
Yellow oil. Bp_{10} 95°.

SH-form

S-Me ester: [2432-83-9].
$C_9H_{18}OS$ M 174.3 Bp_2 85-86°.

S-Et ester: [2432-84-0].
$C_{10}H_{20}OS$ M 188.3 Bp_3 90°.

S-Ph ester: [65842-42-4].
$C_{14}H_{20}OS$ M 236.3 $Bp_{0.1}$ 118-119°.

Fredga, A. *et al*, *Ark. Kemi*, 1950, **2**, 113 (*synth*)
Vinokurov, V.A. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1989, 2154; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1989, 1984 (*S-Me ester, ir, pmr, cmr*)
Katritzky, A.R. *et al*, *Org. Prep. Proced. Int.*, 1995, **27**, 361 (*synth, pmr, cmr*)

1,1,3,3,8,8,10,10-Octaphenyl-1,10-diphospha-3,8-diphosphoniadecane O-1-00024

$Ph_2PCH_2{}^{\oplus}PPh_2(CH_2)_4P^{\oplus}Ph_2CH_2PPh_2$

$C_{54}H_{52}P_4{}^{2\oplus}$ M 824.9 (ion)

Dichloride: [83346-03-6].
$C_{54}H_{52}Cl_2P_4$ M 895.8 Cryst. ($CHCl_3$/Et_2O). Mp 153°.

Dibromide: [83346-02-5].
$C_{54}H_{52}Br_2P_4$ M 984.7 Cryst. (MeOH/Et_2O). Mp 205° dec.

Schmidbaur, H. *et al*, *Z. Naturforsch., B*, 1982, **37**, 677 (*synth*)

2,4,6-Octatriynedioic acid O-1-00025

HOOCC≡CC≡CC≡CCOOH

$C_8H_2O_4$ M 162.1

Dinitrile: [134830-04-9]. *1,6-Dicyano-1,3,5-hexatriyne*
C_8N_2 M 124.1 Formed when graphite is vapourised under cyanogen. Accompanied by smaller amts. of higher homologues. Cryst. Sol. toluene, $CHCl_3$; spar. sol. hexane. Gradually dec. in solid state, can be stored at −18° in soln.

Grosser, T. *et al*, *Angew. Chem., Int. Ed.*, 1993, **32**, 1340.

4-Octene-2,6-diyne, 9CI O-1-00026

[32803-85-3]

$H_3CC{\equiv}CCH{=}CHC{\equiv}CCH_3$

C_8H_8 M 104.1

(E)-form [20060-07-5]
Prisms (pentane). Mp 77-78°. Rapidly dec. on standing.

[159149-26-5]

Sondheimer, F. *et al*, *J.A.C.S.*, 1968, **90**, 4940 (*synth, ir, uv*)
Roth, W.R. *et al*, *Chem. Ber.*, 1994, **127**, 1781 (*pmr, cmr, ir, uv, ms*)

3-Octylamine O-1-00027

3-Octanamine, 9CI. 1-Ethylhexylamine, 8CI. 3-Aminooctane

[24552-04-3]

$H_3C(CH_2)_4CH(NH_2)CH_2CH_3$

$C_8H_{19}N$ M 129.2

(±)-form
Liq. Bp 161-163°, Bp_{16} 57-57.5°.

Hydrochloride: Mp 130°.

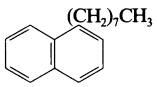
N,N-Di-Me: [24539-82-0].
$C_{10}H_{23}N$ M 157.2 Liq. Bp 186-187°.

Rohrmann, E. *et al*, *J.A.C.S.*, 1944, **66**, 1516 (*synth*)
Geiseler, G. *et al*, *Chem. Ber.*, 1961, **94**, 1008 (*synth*)
Brown, C.A. *et al*, *Org. Mass Spectrom.*, 1969, **2**, 625 (*synth, ms*)
Akermark, B. *et al*, *J. Organomet. Chem.*, 1974, **72**, 127 (*synth, deriv*)

1-Octylnaphthalene O-1-00028

1-(1-Naphthalenyl)octane

[2876-51-9]



$C_{18}H_{24}$ M 240.3
d^{20} 0.942. Fp −2°. Bp 356°, Bp_1 146°. n_D^{20} 1.5526.

Adv. Chem. Ser., 1955, **15**, 228 (***props***)

2-Octylnaphthalene O-1-00029

1-(2-Naphthalenyl)octane

[2876-44-0]

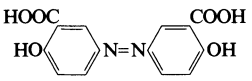
$C_{18}H_{24}$ M 240.3
d^{20} 0.935. Fp 12°. Bp 357°, Bp_1 145-148°. n_D^{20} 1.5501.

Adv. Chem. Ser., 1955, **15**, 228 (***props***)

Olsalazine, BAN, INN O-1-00030

3,3'-Azobis[6-hydroxybenzoic acid], 9CI. 5,5'-Azodisalicylic acid. 4,4'-Dihydroxyazobenzene-3,3'-dicarboxylic acid. C.I. Mordant Yellow S. Azodisal. Dipentum. Procolon. C.I. 14130. CJ 91B

[15722-48-2]



$C_{14}H_{10}N_2O_6$ M 302.2
Dye. Antiinflammatory agent. Used in the treatment of ulcerative colitis. Mp >300°.

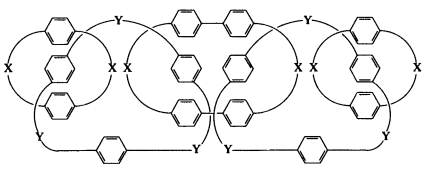
Di-Na salt: [6054-98-4]. ***Olsalazine sodium, BAN, USAN.*** *Sodium azodisalicylate*
Launched 1986.

Di-Ca salt: Green-black powder.

U.K. Pat., 408 676, (1934) (*IG Farben*); *CA*, **28**, 5679 (*synth*)
Henry, R.A., *J.O.C.*, 1958, **23**, 648 (*synth*)
Eur. Pat., 36 637, (1981) (*Pharmacia*); *CA*, **96**, 57761k (*synth, pharmacol*)
U.S. Pat., 4 312 806, (1982) (*GD Searle*); *CA*, **96**, 142468q (*synth, pharmacol, deriv*)

Ryde, M. *et al, Scand. J. Gastroenterol.*, 1983, **18**, 571 (*pharmacol*)
Van Hogezand, R.A. *et al, J. Chromatogr.*, 1984, **305**, 470 (*hplc*)
Carlin, G. *et al, Agents Actions*, 1985, **16**, 377 (*pharmacol*)
Levinson, R.A. *et al, Am. J. Gastroenterol.*, 1985, **80**, 203 (*rev, pharmacol*)
Van Hogezand, R.A. *et al, Gastroenterology*, 1985, **88**, 717 (*pharmacol*)
Fricke, U., *Dtsch. Apoth. -Ztg.*, 1990, **130**, 856 (*rev, pharmacol*)
Thesen, R. *et al, Pharm. Ztg.*, 1990, **135**, 38 (*rev, pharmacol*)
Wadworth, A.N. *et al, Drugs*, 1991, **41**, 647 (*rev*)
Segars, L.W. *et al, Clin. Pharm.*, 1992, **11**, 514 (*rev*)
Scheurlen, C. *et al, Scand. J. Gastroenterol.*, 1992, **27**, 311 (*activity*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 896.

Olympiadane O-1-00031



X = $-H_2C^{\oplus}N$  $N^{\oplus}CH_2-$

Y = $-OCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_2CH_2O-$

$C_{204}H_{224}N_{12}O_{30}^{12\oplus}$ M 3324.0 (ion)
First [5]catenane. Violet solid (as dodekakis(hexafluorophosphate)). Mp >250° (as dodekakis(hexafluorophosphate)).

Amabilino, D.B. *et al, Angew. Chem., Int. Ed.*, 1994, **33**, 1286 (*synth, uv, pmr*)

6-Oxabicyclo[3.1.0]hex-2-ene O-1-00032

3,4-Epoxycyclopentene

C_5H_6O M 82.1

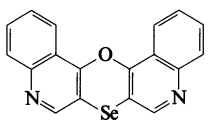
(±)-***form***
Bp_{10-15} 20-26°.

▶ Potentially explosive synth. and dist. of impure material.

Org. Synth., Coll. Vol., 5, 1973, 414 (*synth, haz*)
Merlo, V. *et al, J.C.S. Perkin 1*, 1994, 1477 (*synth, pmr, cmr*)

[1,4]Oxaselenino[3,2-*c*:5,6-*c'*] diquinoline, 9CI O-1-00033

[162469-53-6]



$C_{18}H_{10}N_2OSe$ M 349.2
Plates + 1 H_2O (EtOH). Mp 183-184°.

Löwe, W. *et al, J. Het. Chem.*, 1995, **32**, 271 (*synth, pmr*)

3-Oxetanone, 9CI O-1-00034

[6704-31-0]

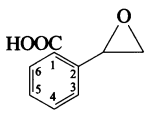
$C_3H_4O_2$ M 72.0
Liq. d_4^{27} 1.137. Bp 106°. n_D^{25} 1.4224. Polym. occurs during storage at r.t.

2,4-Dinitrophenylhydrazone: Pale orange needles. Mp 152-155°.

Marshall, J.R. *et al, J.C.S.*, 1952, 467 (*synth*)
Wojtowicz, J.A. *et al, J.O.C.*, 1973, **38**, 2061 (*synth, ir, pmr*)
Kozikowski, A.P. *et al, Synlett*, 1991, 783 (*synth*)

2-Oxiranylbenzoic acid O-1-00035

2-(Epoxyethyl)benzoic acid



$C_9H_8O_3$ M 164.1

(±)-***form***

Me ester:
$C_{10}H_{10}O_3$ M 178.1 Oil.

Sugimoto, A. *et al, Synthesis*, 1995, 431 (*Me ester*)

3-Oxiranylbenzoic acid O-1-00036

3-(Epoxyethyl)benzoic acid

$C_9H_8O_3$ M 164.1

(±)-***form***

Nitrile: [13906-62-2]. *2-(2-Cyanophenyl) oxirane.* m-*(Epoxyethyl)benzonitrile, 8CI.* m-*Cyanostyrene oxide*
C_9H_7NO M 145.1 Liq. Bp_3 121-123°. n_D^{20} 1.5539.

Barantsevich, E.N. *et al, Zh. Org. Khim.*, 1967, **3**, 110; *J. Org. Chem. USSR (Engl. Transl.)*, 106 (*nitrile*)
Eistert, B. *et al, Chem. Ber.*, 1976, **109**, 640 (*nitrile*)

4-Oxiranylbenzoic acid O-1-00037

4-(Epoxyethyl)benzoic acid

[159262-71-2]

$C_9H_8O_3$ M 164.1

(±)-***form***

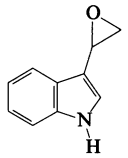
Me ester: [36099-25-9].
$C_{10}H_{10}O_3$ M 178.1 Pale yellow oil.

Nitrile: [52695-39-3]. *(4-Cyanophenyl)oxirane.* p-*(Epoxyethyl)benzonitrile, 8CI.* p-*Cyanostyrene oxide*
C_9H_7NO M 145.1 Mp 34-35°.

Tamura, N. *et al, Chem. Pharm. Bull.*, 1982, **30**, 1393 (*nitrile*)
Ger. Pat., 3 903 988, (1990); *CA*, **114**, 101370y (*Me ester*)

3-Oxiranyl-1*H*-indole, 9CI O-1-00038

3-Indolylethylene oxide

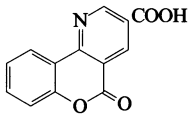


$C_{10}H_9NO$ M 159.1

(−)-***form*** [129225-30-5]
Alkaloid from leaves of *Moricandia arvensis* (Cruciferae). $[\alpha]_D^{22}$ −40 (c, 1 in H_2O).

Belkhiri, A. *et al, Phytochemistry*, 1990, **29**, 1315 (*isol, uv, pmr, ms, struct*)

5-Oxo-5*H*-[1]benzopyrano[4,3-*b*]pyridine-3-carboxylic acid O-1-00039



$C_{13}H_7NO_4$ M 241.2

Me ester:
$C_{14}H_9NO_4$ M 255.2 Cryst. (MeOH). Mp 193-194°.

Et ester:
$C_{15}H_{11}NO_4$ M 269.2 Cryst. (EtOH). Mp 143-144°.

Nitrile:
$C_{13}H_6N_2O_2$ M 222.2 Cryst. (Me_2CO). Mp 246-247°.

Heber, D. *et al, J. Het. Chem.*, 1995, **32**, 505.

2-Oxocyclopentaneacetic acid O-1-00040

[1460-38-4]

(*R*)-*form*

$C_7H_{10}O_3$ M 142.1

(***R***)-***form***
Oil. Bp_2 120°. $[\alpha]_D^{23}$ +127 (c, 1.07 in MeOH).

Me ester: [49826-05-3].
$C_8H_{12}O_3$ M 156.1 $[\alpha]_D$ +123.

(±)-***form*** [104115-44-8]
Mp 53°. Bp_5 170-180°.

Me ester: [135093-95-7].
Bp_{13} 120°, $Bp_{0.03}$ 90-100°. n_D^{20} 1.4570.

Et ester: [104808-87-9].
$C_9H_{14}O_3$ M 170.2 Liq. Bp_{13} 123°, Bp_7 120-130°.

[4934-95-6, 20826-94-2]

Linstead, R.P. *et al, J.C.S.*, 1934, 935 (±-*form*)
Hashimoto, S. *et al, Synth. Commun.*, 1992, **22**, 2722 (*R-form*)

4-Oxo-7-decenoic acid O-1-00041

$H_3CCH_2CH{=}CHCH_2CH_2COCH_2CH_2COOH$

$C_{10}H_{16}O_3$ M 184.2

(***Z***)-***form*** [72049-86-6]
Liq.

Me ester: [85670-53-7].

$C_{11}H_{18}O_3$ M 198.2 $Bp_{0.05}$ 150°.

Matsuda, I. *et al, J.O.C.*, 1980, **45**, 237 (*synth*)
Ballini, R. *et al, Synth. Commun.*, 1989, **19**, 575 (*Me ester*)
Geraghty, N.W.A. *et al, Synth. Commun.*, 1994, **24**, 1351 (*Me ester*)

10-Oxo-8-decenoic acid O-1-00042

9-Formyl-8-nonenoic acid

[79868-90-9]

$OHCCH{=}CH(CH_2)_6COOH$

$C_{10}H_{16}O_3$ M 184.2

(E)-form [69152-89-2]
Constit. of the mushroom *Agaricus bisporus*. Cryst. (EtOAc). Mp 49-51°.

Me ester: [67803-48-9].
$C_{11}H_{18}O_3$ M 198.2 Liq. $Bp_{0.1}$ 108-113°.

(Z)-form [69152-91-6]
Mp 36-40° (impure).

[65114-83-2]

Smith, J.R.L. *et al, Tetrahedron*, 1978, **34**, 1381 (*synth*)
Ranganathan, D. *et al, Tetrahedron*, 1980, **36**, 1869 (*synth, ester*)
Dasaradhi, L. *et al, Synth. Commun.*, 1991, **21**, 183 (*synth, ester*)
Mau, J.L. *et al, Phytochemistry*, 1992, **31**, 4059 (*isol*)

(2-Oxo-1,2-diphenylethyl) phosphonic acid O-1-00043

$PhCOCHPhP(O)(OH)_2$

$C_{14}H_{13}O_4P$ M 276.2

(±)-form

Di-Me ester: Dimethyl (2-oxo-1,2-diphenylethyl)phosphonate
$C_{16}H_{17}O_4P$ M 304.2 Cryst. (butanol). Mp 139.5-140.5°.

Di-Et ester: Diethyl (2-oxo-1,2-diphenylethyl) phosphonate
$C_{18}H_{21}O_4P$ M 332.3 Oil or solid. Mp 175-176°. $Bp_{0.5}$ 184°. n_D^{20} 1.6343.

[22894-32-2, 64196-48-1]

Chiusoli, G.P. *et al, Gazz. Chim. Ital.*, 1977, **107**, 217 (*di-Et ester, synth, ir, ms, pmr*)
Bottin-Strzalko, T. *et al, Bull. Soc. Chim. Fr.*, Part II, 1984, 161 (*di-Et ester, synth, ir, pmr*)
Ronsis, V. *et al, J.O.C.*, 1989, **54**, 627 (*di-Et ester, synth, ms, pmr, cmr*)
Polozov, A.M. *et al, Synthesis*, 1990, 515 (*synth, pmr, P-31 nmr*)
Russell, G.A. *et al, J.O.C.*, 1992, **57**, 6508 (*di-Et ester, synth, ir, ms, pmr, cmr*)

4-Oxododecanoic acid, 9CI O-1-00044

γ-Ketolauric acid

[4144-55-2]

$H_3C(CH_2)_7COCH_2CH_2COOH$

$C_{12}H_{22}O_3$ M 214.3
Needles (heptane). Mp 80-81° (77-78°).

Me ester: [33566-59-5].
$C_{13}H_{24}O_3$ M 228.3 Oil. Bp_2 128-130°.

Et ester: [59941-35-4].
$C_{14}H_{26}O_3$ M 242.3 Oil. Bp_1 126-128°.

Nitrile: [73642-86-1]. *1-Cyano-3-undecanone*
$C_{12}H_{21}NO$ M 195.3 $Bp_{0.1}$ 111°.

Ponomarev, A.A. *et al, Zh. Obshch. Khim.*, 1962, **32**, 2540; *J. Gen. Chem. USSR (Engl. Transl.)*, 1962, 2505 (*synth*)
Smith, R.L. *et al, J. Med. Chem.*, 1977, **20**, 1292 (*synth*)
Zav'yalov, S.I. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1989, 2339; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1989, 2152 (*synth, ir, pmr*)
Geraghty, N.W.A. *et al, Synth. Commun.*, 1994, **24**, 1351 (*Me ester, synth*)

3-Oxoheptanedioic acid, 9CI O-1-00045

[1608-78-2]

$HOOCCH_2CH_2CH_2COCH_2COOH$

$C_7H_{10}O_5$ M 174.1
Mp 70-75° dec.

Di-Me ester: [15890-00-3].
$C_9H_{14}O_5$ M 202.2 $Bp_{0.5}$ 120°.

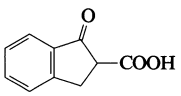
Diethyl ester: [40420-22-2].
$C_{11}H_{18}O_5$ M 230.2 d 1.08. $Bp_{0.5}$ 130-132°.

Aldrich Library of NMR Spectra, 2nd edn., **1**, 583A.
Birkofer, L. *et al, Chem. Ber.*, 1953, **86**, 32 (*synth*)
Thoma, H. *et al, Annalen*, 1983, 1237 (*synth, ir, pmr*)
Celerier, J.P. *et al, J. Het. Chem.*, 1988, **25**, 1275 (*synth, ir*)
Schmidt, H.W. *et al, Org. Prep. Proced. Int.*, 1988, **20**, 184 (*synth*)

1-Oxo-2-indanecarboxylic acid O-1-00046

2,3-Dihydro-1-oxo-1H-indene-2-carboxylic acid, 9CI

[6742-29-6]



$C_{10}H_8O_3$ M 176.1

(±)-form
Cryst. Mp 100-101° dec.

Oxime:
$C_{10}H_9NO_3$ M 191.1 Cryst. Mp 143-144°.

Me ester: [22955-77-7].
$C_{11}H_{10}O_3$ M 190.1 Pale yellow oil.

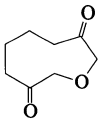
Et ester:
$C_{12}H_{12}O_3$ M 204.2 Oil. Bp_{20} 185°.

Nitrile: 2-Cyano-1-indanone
$C_{10}H_7NO$ M 157.1 Cryst. (EtOH). Mp 68-69°.

[81526-27-4]

Scheiber, J. *et al, Ber.*, 1914, **47**, 3326 (*synth*)
Johnson, W.S. *et al, J.A.C.S.*, 1945, **67**, 1745 (*synth, nitrile*)
Wiley, R.H. *et al, J.A.C.S.*, 1949, **71**, 2429 (*synth*)
Stiles, M., *J.A.C.S.*, 1959, **81**, 2598 (*synth*)
Matsumura, N. *et al, Nippon Kagaku Kaishi*, 1977, 1344 (*synth*)
Brunner, H. *et al, J. Mol. Catal.*, 1989, **49**, 133 (*Me ester*)
Murphy, J.A. *et al, J.C.S. Perkin 1*, 1993, 405 (*Me ester, synth, ir, pmr, cmr, ms*)

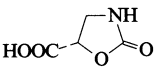
3,8-Oxonanedione O-1-00047



$C_8H_{12}O_3$ M 156.1
Oil.

Brown, D.S. *et al, J.C.S. Perkin 1*, 1995, 1137 (*synth, ir, pmr, cmr, ms*)

2-Oxo-5-oxazolidinecarboxylic acid, 9CI O-1-00048



(S)-form

$C_4H_5NO_4$ M 131.0

(S)-form [81130-97-4]
Mp 59-60°. $[\alpha]_D^{25}$ −6.1 (c, 0.6 in MeOH).

Benzyl ester: [112663-80-6].
$C_{11}H_{11}NO_4$ M 221.2 Cryst. (EtOAc/diisopropyl ether). Mp 128-130°. $[\alpha]_D^{25}$ +3.8 (c, 1.7 in DMF).

(±)-form [60487-08-3]
Cryst. (H_2O). Mp 170-171° dec.

Me ester: [15042-69-0].
$C_5H_7NO_4$ M 145.1 Mp 66-67°.

Nitrile: [15042-67-8]. *2-Oxo-5-oxazolidinecarbonitrile, 8CI. 5-Cyano-2-oxazolidinone*
$C_4H_4N_2O_2$ M 112.0 Cryst. (hexane). Mp 94.5-95.5°.

Gundermann, K.-D. *et al, Chem. Ber.*, 1958, **91**, 160 (*synth, ir*)
Foglia, T.A. *et al, J.O.C.*, 1968, **33**, 766 (*Me ester, nitrile*)
Bal'on, Y.G. *et al, Zh. Org. Khim.*, 1980, **16**, 556; *J. Org. Chem. USSR (Engl. Transl.)*, 1980, **16**, 481 (*Me ester, nitrile*)
Maeda, H. *et al, Synthesis*, 1988, 401 (*benzyl ester*)
Misiti, D. *et al, Synth. Commun.*, 1995, **25**, 2285 (*S-form, synth, ir, pmr, cmr*)

4-Oxopentadecanoic acid, 9CI O-1-00049

[109788-69-4]

$H_3C(CH_2)_{10}COCH_2CH_2COOH$

$C_{15}H_{28}O_3$ M 256.3
Cryst. (hexane or petrol). Mp 92.6°.

Clutterbuck, P.W. *et al, Philos. Trans. R. Soc. London*, 1931, **220B**, 301 (*synth*)
Zav'yalov, S.I. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1987, 667; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1987, 609 (*synth, pmr*)
Ballini, R. *et al, Synthesis*, 1994, 723 (*synth, pmr, ir*)

3-Oxopentanal, 9CI O-1-00050

3-Oxovaleraldehyde, 8CI. 1-Hydroxy-1-penten-3-one

$H_3CCH_2COCH_2CHO \rightleftharpoons H_3CCH_2COCH{=}CHOH$

$C_5H_8O_2$ M 100.1
Exists in the enol form in non polar solvents. Polym. readily at r.t. but fairly stable at −80°.

Oxo-form [623-38-1]

1,1-Dimethyl acetal: [31199-03-8]. *1,1-Dimethoxy-3-pentanone, 9CI*
$C_7H_{14}O_3$ M 146.1 Pale yellow liq. Bp_{10} 83°.

Enol-form [40559-69-1]

Me ether: [65648-57-9]. *1-Methoxy-1-penten-3-one*
$C_6H_{10}O_2$ M 114.1 Oil. Bp_{30} 92-93°.

[42731-24-8, 42731-25-9]

Paterson, T. *et al, J.C.S. Perkin 1*, 1972, 1041 (*synth, pmr, acetal*)
Terpinski, J., *Rocz. Chem.*, 1972, **46**, 1881; 1974, **48**, 1413 (*synth, pmr, tautom*)
Harayama, T. *et al, Chem. Pharm. Bull.*, 1978, **26**, 1201 (*synth, enol ether*)

5-Oxo-2-pentenoic acid, 9CI O-1-00051

γ-Glutaconaldehydic acid. 4-Formylcrotonic acid

[4568-52-9]

$OHCCH_2CH{=}CHCOOH$

$C_5H_6O_3$ M 114.1

Et ester:
$C_7H_{10}O_3$ M 142.1 Yellow oil.

Et ester, 2,4-dinitrophenylhydrazone: Yellow cryst. Mp 147-148°.

Borsche, W. *et al, Annalen*, 1933, **505**, 177 (*synth*)

5-Oxo-3-pentenoic acid, 9CI O-1-00052

α-Glutaconaldehydic acid. 4-Formyl-3-butenoic acid, 8CI

[5809-66-5]

$OHCCH{=}CHCH_2COOH$

$C_5H_6O_3$ M 114.1

(E)-form

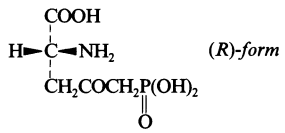
Me ester: [21206-66-6].
$C_6H_8O_3$ M 128.1 Liq. $Bp_{0.005}$ 25°.

Me ester, 2,4-dinitrophenylhydrazone: Cryst. (MeOH aq.). Mp 151-154°.

Pirkle, W.H. *et al, J.A.C.S.*, 1969, **91**, 1179 (*synth, ir, pmr*)

4-Oxo-5-phosphononorvaline, 9CI O-1-00053

2-Amino-4-oxo-5-phosphonopentanoic acid



(*R*)-*form*

$C_5H_{10}NO_6P$ M 211.1

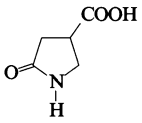
(R)-form [129938-34-7]
Selective glutamate site antagonist of *N*-methyl-D-aspartic acid. Solid. Mp 154° dec. $[\alpha]_D^{20}$ +4.4 (c, 1.0 in H_2O).

(S)-form [83972-10-5]
Solid. Mp 155° dec. Inactive as antagonist.

Eur. Pat., 418 863, (1990); *CA*, **115**, 136385e (*synth, pmr*)
Whitten, J.P. *et al, J. Med. Chem.*, 1990, **33**, 2963 (*synth*)
Rudishill, D.E. *et al, Synthesis*, 1994, 851 (*synth, pmr, cmr, P-31 nmr*)

5-Oxo-3-pyrrolidinecarboxylic acid, 9CI O-1-00054

[7268-43-1]



$C_5H_7NO_3$ M 129.1

(±)-form [64520-51-0]

Me ester: [35309-35-4].
$C_6H_9NO_3$ M 143.1 Liq.

N-*Me:* [42346-68-9]. *1-Methyl-4-carboxy-2-pyrrolidone*
$C_6H_9NO_3$ M 143.1 Cryst. (Me_2CO). Mp 151-153°.

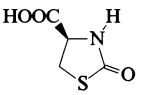
N-*Me, Me ester:* [59857-86-2]. *1-Methyl-4-methoxycarbonyl-2-pyrrolidone*
$C_7H_{11}NO_3$ M 157.1 Oil. Mp 13-17°. $Bp_{0.5}$ 141-144°.

N-*Benzyl, Me ester:* [126344-01-2].
$C_{13}H_{15}NO_3$ M 233.2 Mp 63-66°.

[51535-00-3]

Tsuge, O. *et al, Bull. Chem. Soc. Jpn.*, 1986, **59**, 2537 (*synth, ir, pmr, cmr, ms*)
Sasaki, H. *et al, Int. J. Pharm.*, 1988, **44**, 15 (*N-Me derivs, synth, pmr*)

2-Oxo-4-thiazolidinecarboxylic acid O-1-00055



$C_4H_5NO_3S$ M 147.1

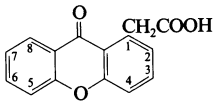
(S)-form
L-*form*
Cubes (H_2O). Sol. EtOH; insol. C_6H_6, EtOAc. Mp 171-173° dec. $[\alpha]_D^{20}$ −59.4 (c, 2 in H_2O).

Maclaren, J.A., *Aust. J. Chem.*, 1968, **21**, 1891 (*synth*)
Keszler, D.A. *et al, Acta Cryst. C*, 1991, **47**, 1481 (*cryst struct*)

9-Oxo-9*H*-xanthene-1-acetic acid, 9CI O-1-00056

Xanthone-1-acetic acid

[59292-04-5]



$C_{15}H_{10}O_4$ M 254.2
Cryst. Mp 252-254°.

Nitrile: [59292-12-5]. *1-(Cyanomethyl) xanthone*
$C_{15}H_9NO_2$ M 235.2 Mp 180-190°.

[59292-16-9, 88521-86-2]

Rewcastle, G.W. *et al, J. Med. Chem.*, 1989, **32**, 793 (*synth*)

9-Oxo-9*H*-xanthene-2-acetic acid, 9CI O-1-00057

Xanthone-2-acetic acid

[30087-31-1]

$C_{15}H_{10}O_4$ M 254.2
Cryst. Mp 224-226°.

Nitrile: [30087-35-5]. *2-(Cyanomethyl) xanthone*
$C_{15}H_9NO_2$ M 235.2 Mp 190-191°.

[78096-25-0]

Marona, H. *et al, Pol. J. Chem.* (*Rocz. Chem.*), 1980, **54**, 2059 (*synth*)
Rewcastle, G.W. *et al, J. Med. Chem.*, 1989, **32**, 793 (*synth*)

9-Oxo-9*H*-xanthene-3-acetic acid, 9CI O-1-00058

Xanthone-3-acetic acid

[118537-75-0]

$C_{15}H_{10}O_4$ M 254.2
Cryst. Mp 149-150°.

Nitrile: [118537-82-9]. *3-(Cyanomethyl) xanthone*
$C_{15}H_9NO_2$ M 235.2 Mp 149-150°.

Rewcastle, G.W. *et al, J. Med. Chem.*, 1989, **32**, 793 (*synth*)

3,3′-Oxybis[2,2-dimethylpropanoic acid], 9CI O-1-00059

2,2,6,6-Tetramethyl-4-oxaheptanedioic acid

[13987-64-9]

$HOOCC(CH_3)_2CH_2OCH_2C(CH_3)_2COOH$

$C_{10}H_{18}O_5$ M 218.2
Cryst. (AcOH/petrol). Mp 134-135°.

Di-Et ester: [34506-36-0].
$C_{14}H_{26}O_5$ M 274.3 Liq. $Bp_{0.1}$ 73-75°.

Dinitrile: [152405-31-7].
$C_{10}H_{16}N_2O$ M 180.2 Cryst.

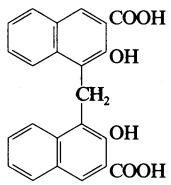
Johnson, P.Y. *et al, J.O.C.*, 1973, **38**, 2346 (*synth, ir, pmr, ms*)
Isaksson, R. *et al, J.C.S. Perkin 2*, 1983, 1351 (*synth*)
Ferguson, G. *et al, Acta Cryst. C*, 1994, **50**, 77 (*cryst struct, dinitrile*)

P

Pamoic acid P-1-00001

4,4'-Methylenebis[3-hydroxy-2-naphthalenecarboxylic acid], 9CI

[130-85-8]



$C_{23}H_{16}O_6$ M 388.3

Used to prepare pamoate salts for administration of basic drugs. Cryst.

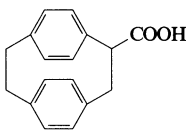
Barber, H.J. *et al, J. Appl. Chem.*, 1952, **2**, 565 (*synth*)

Kondekar, N. *et al, Ind. Eng. Chem. Process Des. Dev.*, 1973, **12**, 135 (*synth*)

[2.2]Paracyclophane-1-carboxylic acid P-1-00002

Tricyclo[8.2.2.2^{4,7}]hexadeca-4,6,10,12,13,15-hexaene-2-carboxylic acid, 9CI

[10181-82-5]



$C_{17}H_{16}O_2$ M 252.3

(+)-***form*** [32212-99-0]
Mp 187-188°. $[\alpha]_{546}^{25}$ +42.0 (c, 0.56 in $CHCl_3$).

Me ester: [32213-00-6].
$C_{18}H_{18}O_2$ M 266.3 Mp 115.5-116.5°. $[\alpha]_{546}^{25}$ +49.2 (c, 0.6 in $CHCl_3$).

(−)-***form*** [32221-47-9]
Mp 187-188°. $[\alpha]_{546}^{25}$ −44.1 (c, 0.54 in $CHCl_3$).

Me ester: Mp 115.5-116.5°. $[\alpha]_{546}^{25}$ −51.2 (c, 0.5 in $CHCl_3$).

(±)-***form***
Cryst. (EtOH). Mp 187-188°.

Me ester: [32212-98-9].
Cryst. (hexane). Mp 96.5-97.5°.

Nitrile: [100703-43-3]. *1-Cyano[2.2]paracyclophane*
$C_{17}H_{15}N$ M 233.3 Needles. Mp 131°.

Hedaya, E. *et al, J.O.C.*, 1967, **32**, 197 (*synth, Me ester*)

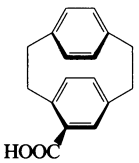
Cram, D.J. *et al, J.A.C.S.*, 1970, **92**, 7623; 1972, **94**, 2471 (*synth, Me ester*)

Hopf, H. *et al, Chem. Ber.*, 1986, **119**, 1836 (*nitrile*)

[2.2]Paracyclophane-4-carboxylic acid P-1-00003

Tricyclo[8.2.2.2^{4,7}]hexadeca-4,6,10,12,13,15-hexaene-5-carboxylic acid, 9CI

[18931-39-0]



(*R*)-*form*

$C_{17}H_{16}O_2$ M 252.3

(***R*)-*form*** [108340-94-9]
Plates (AcOH). Mp 211.5-213°. $[\alpha]_D^{20}$ −175 (c, 0.68 in $CHCl_3$).

Amide: [28908-13-6].
$C_{17}H_{17}NO$ M 251.3 Needles ($CHCl_3$). Mp 179-181°. $[\alpha]_D^{21}$ −135.5 (c, 1 in $CHCl_3$).

(***S*)-*form*** [19776-83-1]
Plates (AcOH). Mp 212-214°. $[\alpha]_D^{20}$ +170 (c, 0.5 in $CHCl_3$).

(±)-***form*** [20586-49-6]
Needles (AcOH aq.). Mp 223.5-224.5°.

Me ester: [147049-45-4].
$C_{18}H_{18}O_2$ M 266.3 Mp 132°.

Amide: [28908-14-7].
Cubes. Mp 215-216.5°.

Nitrile: 4-Cyano[2.2]paracyclophane
$C_{17}H_{15}N$ M 233.3 Cryst. ($CHCl_3$). Mp 123-124°.

[1438-68-2, 10029-01-3]

Cram, D.J. *et al, J.A.C.S.*, 1955, **77**, 6289; 1963, **85**, 1075 (*synth, amide, nitrile*)

Matsuo, H. *et al, Chem. Pharm. Bull.*, 1970, **18**, 1693 (*amide, synth*)

Falk, H. *et al, Tetrahedron*, 1970, **26**, 511 (*abs config*)

Marshall, J.L. *et al, Tetrahedron*, 1981, **37**, 1271 (*synth*)

Tochtermann, W. *et al, Chem. Ber.*, 1987, **120**, 1523 (*abs config*)

Sutler, J.K. *et al, J. Polym. Sci., Part A: Polym. Chem.*, 1991, **29**, 1917 (*synth, pmr, cmr*)

Ernst, L., *Annalen*, 1995, 13 (*nitrile, conformn*)

1-Pentacontanol P-1-00004

Acalyphol

[40710-43-8]

$H_3C(CH_2)_{48}CH_2OH$

$C_{50}H_{102}O$ M 719.3

Ac: [112515-71-6]. ***Acalyphol acetate***
$C_{52}H_{104}O_2$ M 761.3 Constit. of the leaves of *Acalypha indica*. Mp 75-76°.

Dawson, I.M. *et al, Proc. R. Soc. London*, Ser. A, 1957, **239**, 349.

Ral, A. *et al, Chem. Scr.*, 1973, **3**, 125 (*ms*)

Manzoor-i-Khuda, M. *et al, Bangladesh J. Sci. Ind. Res.*, 1985, **20**, 171 (*isol, acetate*)

1,16-Pentacosadiene P-1-00005

[99461-72-0]

$H_3C(CH_2)_7CH{=}CH(CH_2)_{13}CH{=}CH_2$

$C_{25}H_{48}$ M 348.6

(***E*)-*form*** [104899-44-7]
Isol. from the green alga *Botryococcus braunii*.

(***Z*)-*form*** [104899-39-0]
Isol. from *B. braunii*.

Metzger, P. *et al, Phytochemistry*, 1986, **25**, 1869; 1993, **33**, 1125 (*isol, pmr, cmr*)

7,11-Pentacosadiene P-1-00006

[100462-57-5]

$H_3C(CH_2)_{12}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_5CH_3$

$C_{25}H_{48}$ M 348.6

(***Z,Z*)-*form*** [127599-39-7]
Pheromone of *Drosophila melanogaster*. Oil.

Davis, T.L. *et al, Synthesis*, 1989, 936 (*synth*)

1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-Pentacosafluoro-12-iodododecane, 9CI P-1-00007

Pentacosafluoro-1-iododecane, 8CI. Perfluorododecyl iodide

[307-60-8]

$F_3C(CF_2)_{10}CF_2I$

$C_{12}F_{25}I$ M 745.9
Mp 99-101°. Bp_{18} 108-110°.

Aldrich Library of FT-IR Spectra, 1st edn., **1**, 92B.

Haszeldine, R.N., *J.C.S.*, 1953, 3761 (*synth*)

1-Pentacosene P-1-00008

[16980-85-1]

$H_3C(CH_2)_{22}CH{=}CH_2$

$C_{25}H_{50}$ M 350.6
Isol. from the alga *Botryococcus braunii* and various plant spp. Fp 48.7°. Bp_{30} 271.2°.

Dreisbach, R.R., *Adv. Chem. Ser.*, 1959, **22**, 390 (*props*)

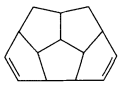
MacLeod, G., *Phytochemistry*, 1990, **29**, 1197 (*isol*)

Metzger, P., *Phytochemistry*, 1993, **33**, 1125 (*isol*)

Pentacyclo [5.4.2^{1,7}.1^{3,6}.0^{10,13}.0^{12,14}] tetradeca-4,8-diene P-1-00009

1,1a,3a,3b,5a,5b,6,6a,6b,6c-Decahydrocyclopenta[cd]pentaleno[2,1,6-gha] pentalene, 9CI

[155787-78-3]



$C_{14}H_{16}$ M 184.2

Cryst. Mp 102-104°. Unstable in air. The cryst. struct. detn. was on a tetrabromo deriv.

Mitsudo, T. *et al, Chem. Comm.*, 1994, 435 (*synth, ir, pmr, cmr, cryst struct*)

3,6-Pentadecadien-1-ol P-1-00010

$H_3C(CH_2)_7CH{=}CHCH_2CH{=}CHCH_2CH_2OH$

$C_{15}H_{28}O$ M 224.3

(3Z,6Z)-form [130727-72-9]

Oil.

Datcheva, V.K. *et al, J.A.C.S.*, 1991, **113**, 270 (*synth, ir, pmr, cmr*)

Butler, P.I. *et al, J.C.S. Perkin 1*, 1994, 1503 (*synth, pmr*)

1,15-Pentadecanediol, 9CI P-1-00011

[14722-40-8]

$HOCH_2(CH_2)_{13}CH_2OH$

$C_{15}H_{32}O_2$ M 244.4

Cryst. (C_6H_6). Mp 87-88°.

Chuit, P. *et al, Helv. Chim. Acta*, 1926, **9**, 264; 1929, **12**, 850 (*synth*)

U.K. Pat., 803 178, (1959); *CA*, **53**, 6985g (*synth*)

Polyakova, S.G. *et al, Zh. Obshch. Khim.*, 1964, **34**, 565; *J. Gen. Chem. USSR (Engl. Transl.)*, 1964, 566 (*synth*)

1-Pentadecyne, 9CI P-1-00012

[765-13-9]

$H_3C(CH_2)_{12}C{\equiv}CH$

$C_{15}H_{28}$ M 208.3

Oil. d_4^{20} 0.83. Mp 15°. Bp_{30} 158°. n_D^{20} 1.4422.

Ryden, L.L. *et al, J.A.C.S.*, 1937, **59**, 1014 (*synth*)

Elsner, B.B. *et al, J.C.S.*, 1951, 893 (*synth*)

Gigg, J. *et al, J.C.S.(C)*, 1966, 1882 (*synth*)

Gal, A.E., *J. Labelled Compd.*, 1967, **3**, 112 (*synth, ir*)

Feldhues, M. *et al, Tetrahedron*, 1985, **41**, 4213 (*synth, ir, pmr, ms*)

10-Pentadecyn-1-ol, 9CI P-1-00013

[68381-03-3]

$H_3C(CH_2)_3C{\equiv}C(CH_2)_8CH_2OH$

$C_{15}H_{28}O$ M 224.3

Oil. $Bp_{2.25}$ 150-152°. n_D^{23} 1.4615.

Ebata, T. *et al, Agric. Biol. Chem.*, 1979, **43**, 1567 (*synth, ir, pmr*)

Svirskaya, P. *et al, J. Chem. Eng. Data*, 1979, **24**, 152 (*synth, ir, pmr*)

Hoskovec, M. *et al, Coll. Czech. Chem. Comm.*, 1990, **55**, 2270 (*synth, pmr, cmr*)

Pfeifer, J. *et al, Annalen*, 1995, 131 (*synth, ir, pmr, cmr*)

(Pentafluorophenoxy)acetic acid, 9CI, 8CI P-1-00014

[14892-14-9]

$(C_6F_5)OCH_2COOH$

$C_8H_3F_5O_3$ M 242.1

Cryst. (petrol). Mp 108-110°.

Benzylthiouronium salt: Cryst. (EtOH). Mp 168-169°.

Me ester: [21417-50-5].

$C_9H_5F_5O_3$ M 256.1 Bp_5 97-99°.

Et ester:

$C_{10}H_7F_5O_3$ M 270.1 $Bp_{0.1}$ 56-57°.

Brooke, G.M. *et al, J.C.S.(C)*, 1967, 869 (*synth*)

Abezgauz, F.I. *et al, Zh. Obshch. Khim.*, 1968, **38**, 2502; *J. Gen. Chem. USSR (Engl. Transl.)*, 1968, **38**, 2418 (*synth*)

Mak, T.C.W. *et al, Aust. J. Chem.*, 1988, **41**, 683 (*synth, cryst struct*)

2,2,3,3,3-Pentafluoro-1-phenyl-1-propanone P-1-00015

Pentafluoroethyl phenyl ketone. Benzoylpentafluoroethane

[394-52-5]

$PhCOCF_2CF_3$

$C_9H_5F_5O$ M 224.1

d_4^{25} 1.37. Bp 161°. n_D^{25} 1.4245.

2,4-Dinitrophenylhydrazone: Mp 119-120° (111.8-112.4°).

Simons, J.H. *et al, J.A.C.S.*, 1953, **75**, 5621 (*synth*)

McBee, E.T. *et al, J.A.C.S.*, 1955, **77**, 917 (*synth*)

Dishart, K.T. *et al, J.A.C.S.*, 1956, **78**, 2268 (*synth*)

Griffin, C.E., *Spectrochim. Acta*, 1960, **16**, 1464 (*ir*)

2-(Pentafluorophenyl)ethanol P-1-00016

2,3,4,5,6-Pentafluorobenzeneethanol, 9CI. 2,3,4,5,6-Pentafluorophenethyl alcohol, 8CI

[653-31-6]

$(C_6F_5)CH_2CH_2OH$

$C_8H_5F_5O$ M 212.1

Bp_{16} 104°. n_D^{20} 1.4508.

3,5-Dinitrobenzoyl: Cryst. (EtOH). Mp 94-95°.

Barbour, A.K. *et al, J.C.S.*, 1961, 808.

Vorozhtsov, N.N. *et al, Tet. Lett.*, 1964, 3575 (*synth, uv*)

3-(Pentafluorophenyl) propanoic acid P-1-00017

2,3,4,5,6-Pentafluorobenzenepropanoic acid. 2,3,4,5,6-Pentafluorohydrocinnamic acid

[2002-94-0]

$(C_6F_5)CH_2CH_2COOH$

$C_9H_5F_5O_2$ M 240.1

Cryst. (H_2O). Mp 95-96°.

Brooke, G.M. *et al, J.C.S.*, 1961, 808 (*synth*)

Fuchikami, T. *et al, J.O.C.*, 1983, **48**, 3803 (*synth, pmr, ir, ms, F-19 nmr*)

2,2,3,3,3-Pentafluoro-1-propylamine P-1-00018

3-Amino-1,1,1,2,2-pentafluoropropane

[422-03-7]

$F_3CCF_2CH_2NH_2$

$C_3H_4F_5N$ M 149.0

d 1.40. Bp 49-50° (38°). n_D^{20} 1.297.

Hydrochloride: [374-14-1].

Mp 248°.

N-*Formyl:*

$C_4H_4F_5NO$ M 177.0 d 1.47. Bp_8 81-83°. n_D^{25} 1.3439.

Husted, D.R. *et al, J.A.C.S.*, 1953, **75**, 1605 (*synth*)

Haszeldine, R.N. *et al, J.C.S.*, 1953, 1548 (*synth*)

Dannley, R.L. *et al, J.O.C.*, 1956, **21**, 1318 (*deriv*)

Cohen, W.V., *J.O.C.*, 1961, **26**, 4021 (*synth*)

Pentafluorovinylbenzene P-1-00019

Ethenylpentafluorobenzene, 9CI. 2,3,4,5,6-Pentafluorostyrene, 8CI

[653-34-9]

$(C_6F_5)CH{=}CH_2$

$C_8H_3F_5$ M 194.1

d 1.41. Bp 140-141°, Bp_{50} 62-63°. n_D^{20} 1.45.

[64253-83-4, 102685-91-6]

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 953A.

Aldrich Library of NMR Spectra, 2nd edn., **1**, 818C.

Nield, E. *et al, J.C.S.*, 1959, 166 (*synth*)

Bruce, M.I., *J.C.S.(A)*, 1968, 1459 (*F-19 nmr*)

Green, J.H.S. *et al, Spectrochim. Acta A*, 1977, **33**, 423 (*ir, Raman*)

Nyquist, R.A., *Appl. Spectrosc.*, 1986, **40**, 196 (*ir*)

Rempel, D.L. *et al, Anal. Chem.*, 1989, **61**, 749 (*ms*)

2-Pentanethiol, 9CI P-1-00020

2-Mercaptopentane

[2084-19-7]

$H_3CCH_2CH_2CH(SH)CH_3$

$C_5H_{12}S$ M 104.2

(±)-form

Liq. Bp 112°.

Levene, P.A. *et al, J. Biol. Chem.*, 1927, **75**, 593 (*synth*)

Levy, E.J. *et al, Anal. Chem.*, 1961, **33**, 707 (*ms*)

3-Pentanethiol P-1-00021

3-Mercaptopentane

[616-31-9]

$(H_3CCH_2)_2CHSH$

$C_5H_{12}S$ M 104.2

Liq. Bp 112-113°.

Asinger, F. *et al, Annalen*, 1959, **627**, 195 (*synth*)

Levy, E.C. *et al, Anal. Chem.*, 1961, **33**, 707 (*ms*)

Broer, W.J. *et al, Org. Mass Spectrom.*, 1979, **14**, 36 (*synth*)

Pentaphenyltriphosphine, 9CI, 8CI P-1-00022

[5748-54-9]

$PhP(PPh_2)_2$

$C_{30}H_{25}P_3$ M 478.4
Ligand for Fe, Mo, Pt. Cryst. (Et_2O). Mp 95-96°.

Schumann, H. *et al*, *J. Organomet. Chem.*, 1970, **24**, 183 (*synth, ir, Raman*)

2-Pentene-1,5-diol P-1-00023

$HOCH_2CH_2CH{=}CHCH_2OH$

$C_5H_{10}O_2$ M 102.1

(E)-form
$Bp_{0.07}$ 86°. May cont. (*Z*)-isomer.

(Z)-form [27354-43-4]
Oil.

Bajorek, J.J.S. *et al*, *J.C.S. Perkin 1*, 1974, 1243 (*E-form*)
Procopiou, P.A. *et al*, *J.C.S. Perkin 1*, 1994, 1773 (*Z-form*)

2-Pentenyltriphenylphosphonium(1+) P-1-00024

$Ph_3P^{\oplus}CH_2CH{=}CHCH_2CH_3$

$C_{23}H_{24}P^{\oplus}$ M 331.4 (ion)

(E)-form

Bromide: [7348-72-3].
$C_{23}H_{24}BrP$ M 411.3 Solid. Mp 198-200°.

(Z)-form

Bromide: [7348-79-0].
Cryst. (CH_2Cl_2/C_6H_6). Mp 160-163°.

Daradics, L. *et al*, *J. Prakt. Chem.*, 1987, **329**, 277 (*synth, ir, use*)
Ideses, R. *et al*, *Tetrahedron*, 1989, **45**, 3523 (*synth, pmr*)

3-Pentenyltriphenylphosphonium(1+) P-1-00025

$Ph_3P^{\oplus}CH_2CH_2CH{=}CHCH_3$

$C_{23}H_{24}P^{\oplus}$ M 331.4 (ion)

(E)-form

Bromide: [53143-96-7].
$C_{23}H_{24}BrP$ M 411.3 Solid. Mp 124°.
With $Me_3SiNa \rightarrow$ylide, synth. in situ.

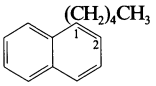
[120593-09-1]

Bestmann, H.J. *et al*, *Annalen*, 1982, 536.

1-Pentylnaphthalene P-1-00026

1-Amylnaphthalene. 1-(1-Naphthalenyl) pentane

[86-89-5]



$C_{15}H_{18}$ M 198.3
Liq. d^{20} 0.966. Fp −22°. Bp 307°, Bp_1 112°. n_D^{23} 1.5725.

Adv. Chem. Ser., 1955, **15**, 222 (***props***)

2-Pentylnaphthalene P-1-00027

2-Amylnaphthalene. 1-(2-Naphthalenyl) pentane

[93-22-1]

$C_{15}H_{18}$ M 198.3
Liq. d^{20} 0.956. Fp −4°. Bp 310°, Bp_1 113.2°. n_D^{20} 1.5694.

Adv. Chem. Ser., 1955, **15**, 223 (***props***)

Pentyl nitrate P-1-00028

[1002-16-0]

$H_3C(CH_2)_4ONO_2$

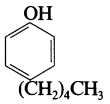
$C_5H_{11}NO_3$ M 133.1
Liq. d_4^{20} 0.996. Bp 157°, Bp_{70} 74-76°.

Suzuki, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 65 (*ms*)
Olah, G.A. *et al*, *Synthesis*, 1993, 207 (*synth, cmr*)

4-Pentylphenol, 9CI P-1-00029

p-Amylphenol

[14938-35-3]



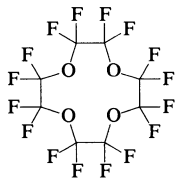
$C_{11}H_{16}O$ M 164.2
Liq. Fp 23°. Bp 250.5°, Bp_1 83.3°. n_D^{20} 1.5272.

Sondulesco, G. *et al*, *Bull. Soc. Chim. Fr.*, 1930, **47**, 1300 (*synth*)
Niederl, J.B. *et al*, *J.A.C.S.*, 1937, **54**, 1113 (*synth*)
Adv. Chem. Ser., 1955, **15**, 298 (***props***)
Ivanovskaya, L.Yu. *et al*, *Zh. Org. Khim.*, 1968, **4**, 1227; *CA*, **69**, 106079x (*synth*)
Gorfinkel, M. *et al*, *Org. Mass Spectrom.*, 1969, **2**, 273 (*ms*)

Perfluoro-12-crown-4 P-1-00030

2,2,3,3,5,5,6,6,8,8,9,9,11,11,12,12-Hexadecafluoro-1,4,7,10-tetraoxacyclododecane, 9CI. Hexadecafluoro-12-crown-4

[97571-68-1]



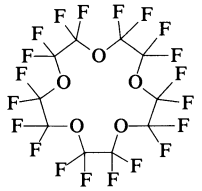
$C_8F_{16}O_4$ M 464.0
Fp −64°. Bp 118°.

Lin, W.-H. *et al*, *Pure Appl. Chem.*, 1988, **60**, 473 (*synth, F-19 nmr, cmr, ms, ir*)
Lin, T.Y. *et al*, *J.A.C.S.*, 1994, **116**, 5172 (*synth, cmr, F-19 nmr, ms*)

Perfluoro-15-crown-5 P-1-00031

2,2,3,3,5,5,6,6,8,8,9,9,11,11,12,12,14,14,15,15-Eicosafluoro-1,4,7,10,13-pentaoxacyclopentadecane, 9CI. Eicosafluoro-15-crown-5. Icosafluoro-15-crown-5

[97571-69-2]

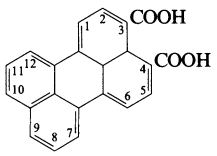


$C_{10}F_{20}O_5$ M 580.0
Fp −11.5°. Bp 146°.

Lin, W.-H. *et al*, *Pure Appl. Chem.*, 1988, **60**, 473 (*synth, F-19 nmr, cmr, ir, ms*)
Lin, T.Y. *et al*, *J.A.C.S.*, 1994, **116**, 5172 (*synth, cmr, F-19 nmr, ms*)

3,4-Perylenedicarboxylic acid, 9CI P-1-00032

[165261-56-3]



$C_{22}H_{12}O_4$ M 340.3
Cryst. (as di-K salt). Mp >250° (di-K salt). Salts and esters display strong solid-state fluorescence.

Di-Me ester: [165261-55-2].
$C_{24}H_{16}O_4$ M 368.3 Yellow-orange powder. Mp 256-257°.

Dipropyl ester:
$C_{28}H_{24}O_4$ M 424.4 Yellow cryst. Mp 253°.

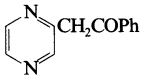
Anhydride: [117364-74-6]. *1H,3H-Perylo[3,4-cd]pyran-1,3-dione, 9CI*
$C_{22}H_{10}O_3$ M 322.3 Red solid. Mp >260°.

Feiler, L. *et al*, *Annalen*, 1995, 1229.

Phenacylpyrazine P-1-00033

1-Phenyl-2-pyrazinylethanone, 9CI. (Benzoylmethyl)pyrazine

[40061-45-8]

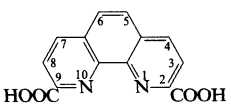


$C_{12}H_{10}N_2O$ M 198.2
Mp 82-83°.

Behun, J.D. *et al*, *J.A.C.S.*, 1959, **81**, 5157 (*synth*)
More O'Ferrall, R.A. *et al*, *J.C.S. Perkin 2*, 1994, 2461, 2471 (*pmr, cmr, tautom*)

1,10-Phenanthroline-2,9-dicarboxylic acid P-1-00034

[57709-61-2]



$C_{14}H_8N_2O_4$ M 268.2
Photosensitizer.

Monohydrate: Mp 238° dec.

Dichloride: [84670-37-1].
$C_{14}H_6Cl_2N_2O_2$ M 305.1 Yellow solid (toluene). Mp 227-228° dec.

Diamide: [145058-23-7].
$C_{14}H_{10}N_4O_2$ M 266.2 Light yellow solid. Mp >300°.

Dinitrile: [57709-63-4]. *2,9-Dicyano-1,10-phenanthroline*
$C_{14}H_6N_4$ M 230.2 Mp >300°.

Deady, L.W. *et al, J. Het. Chem.*, 1981, **18**, 599 (*synth, ir, ms, pmr, C-13 nmr*)
Mäkelä, M. *et al, Synth. Commun.*, 1992, **22**, 2811 (*diamide, dinitrile*)

1,10-Phenanthroline-4,7-dicarboxylic acid P-1-00035

[31301-31-2]

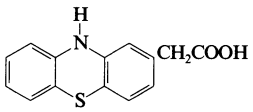
$C_{14}H_8N_2O_4$ M 268.2
Cryst. Not characterised.

Di-Me ester: [142593-09-7].
$C_{16}H_{12}N_2O_4$ M 296.2 Yellow plates + $1H_2O$ (EtOH). Mp 213-214°.

Czuchajowski, L. *et al, J. Het. Chem.*, 1991, **28**, 7 (*synth*)

10*H*-Phenothiazine-2-acetic acid, 9CI P-1-00036

[20965-69-9]



$C_{14}H_{11}NO_2S$ M 257.3
Cryst. (EtOH). Mp 156-157°.

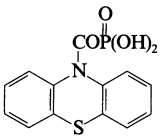
Me ester: [25238-71-5].
$C_{15}H_{13}NO_2S$ M 271.3 Small light-yellow cryst. (MeOH). Mp 106-108°.

N-*Me:* [13993-65-2]. *10-Methyl-10H-phenothiazine-2-acetic acid, 9CI.* ***Metiazinic acid, INN, JAN.*** *Ambrunate. Novartril. RP 16091. Many other names*
$C_{15}H_{13}NO_2S$ M 271.3
Antiinflammatory, analgesic, antirheumatic. Mp 146°.
▶ LD_{50} (rat, orl) 495 mg/kg. Exp. reprod. and teratogenic effects. SN5100000.

Massie, S.P. *et al, J.O.C.*, 1956, **21**, 1006 (*synth*)
Julou, L. *et al, Arzneim.-Forsch.*, 1969, **19**, 1193, 1198, 1207, 12 (*Metiazinic acid*)
Juby, P.F. *et al, Annu. Rep. Med. Chem.*, 1972, 7, 208 (*Metiazinic acid, rev*)
Kitagawa, H. *et al, Jpn. J. Pharmacol.*, 1975, **25**, 1 (*Metiazinic acid*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 24.
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 7th edn., Akademie-Verlag, Berlin, 1994, 4430 (*synonyms*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th Ed., Van Nostrand-Reinhold, 1992, MNQ500.

(10-Phenothiazinecarbonyl)phosphonic acid P-1-00037

(*10H-Phenothiazin-10-ylcarbonyl*)*phosphonic acid*



$C_{13}H_{10}NO_4PS$ M 307.2

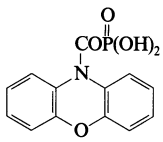
Di-Me ester: [39593-77-6]. *Dimethyl (10-phenothiazinecarbonyl)phosphonate*
$C_{15}H_{14}NO_4PS$ M 335.3 Cryst. (petrol). Mp 113-114°.

Di-Et ester: [39593-78-7]. *Diethyl (10-phenothiazinecarbonyl)phosphonate*
$C_{17}H_{18}NO_4PS$ M 363.3 Cryst. (petrol). Mp 127-128°.

Yarmukhametova, D.Kh. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1972, 2634; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1972, 2652.

(10-Phenoxazinecarbonyl)phosphonic acid P-1-00038

(*10H-Phenoxazin-10-ylcarbonyl*)*phosphonic acid*



$C_{13}H_{10}NO_5P$ M 291.1

Di-Me ester: [39593-72-1]. *Dimethyl (10-phenoxazinecarbonyl)phosphonate*
$C_{15}H_{14}NO_5P$ M 319.2 Cryst. Mp 80-82°.

Di-Et ester: [39593-73-2]. *Diethyl (10-phenoxazinecarbonyl)phosphonate*
$C_{17}H_{18}NO_5P$ M 347.3 Cryst. Mp 114-115°.

Dipropyl ester: [39593-74-3]. *Dipropyl (10-phenoxazinecarbonyl)phosphonate*
$C_{19}H_{22}NO_5P$ M 375.3 Cryst. Mp 64-66°.

Diisopropyl ester: [39593-75-4]. *Diisopropyl (10-phenoxazinecarbonyl)phosphonate*
$C_{19}H_{22}NO_5P$ M 375.3 Cryst. Mp 88-89°.

Yarmukhametova, D.Kh. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1972, 2364; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1972, 2652 (*synth, ir*)

(2-Phenoxyethenyl)phosphonous acid, 9CI P-1-00039

2-Phenoxyvinylphosphonous acid

$PhOCH{=}CHP(OH)_2$

$C_8H_9O_3P$ M 184.1

Di-Et ester: [37916-80-6]. *Diethyl (2-phenoxyethenyl)phosphonite*
$C_{12}H_{17}O_3P$ M 240.2 Liq. d_4^{20} 1.06. $Bp_{2.5}$ 107-108°. n_D^{20} 1.5228.

Dichloride: [21722-84-9].
$C_8H_7Cl_2OP$ M 221.0 Liq. d_4^{20} 1.30. Bp_3 93-99°, Bp_2 150-152°. n_D^{20} 1.5976.

Foss, V.L. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1962, **146**, 1106; *Dokl. Chem.* (*Engl. Transl.*), 1962, **146**, 906.
Ratovskii, G.V. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1970, **190**, 1124; *Dokl. Chem.* (*Engl. Transl.*), 1970, **190**, 147 (*ir*)
Dorokhova, V.V. *et al, Zh. Obshch. Khim.*, 1973, **43**, 2172; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1973, **43**, 2164 (*dichloride, uv, Raman, theory*)
Rozinov, V.G. *et al, Zh. Obshch. Khim.*, 1982, **52**, 1994; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1982, **52**, 1772 (*dichloride, synth, P-31 nmr*)
Timokhin, B.V. *et al, Zh. Obshch. Khim.*, 1983, **53**, 291; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1983, **53**, 252 (*dichloride, synth, pmr, P-31 nmr*)

2-(Phenylacetyl)furan P-1-00040

1-(2-Furanyl)-2-phenylethanone

$C_{12}H_{10}O_2$ M 186.2
Mp 47° (40°). pK_a 14.38 (25°, NaOH aq.).

Borsche, W. *et al, Ber.*, 1938, **71**, 957.
Fontana, A. *et al, J.C.S. Perkin 2*, 1994, 2453 (*synth, pmr, tautom*)

(Phenylacetyl)phosphonic acid P-1-00041

(*1-Oxo-2-phenylethyl*)*phosphonic acid, 9CI. Phenacetylphosphonic acid*

[67532-95-0]

$PhCH_2COP(O)(OH)_2$

$C_8H_9O_4P$ M 200.1
Visc. oil.

Di-Me ester: [51463-66-2]. *Dimethyl (phenylacetyl)phosphonate*
$C_{10}H_{13}O_4P$ M 228.1 Liq. $Bp_{0.1}$ 125°.

Di-Me ester, 4-methylbenzenesulfonylhydrazone: Solid. Mp 125-126°.

Diisopropyl ester, oxime:
$C_{14}H_{22}NO_4P$ M 299.3 Cryst. (CCl_4/hexane). Mp 95-96°.

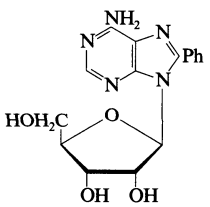
Dibenzyl ester: Dibenzyl (phenylacetyl) phosphonate
$C_{22}H_{21}O_4P$ M 380.3 Cryst. (CCl_4). Mp 118-119°.

Dibenzyl ester, 2,4-dinitrophenylhydrazone: Solid. Mp 107-109°, Mp 126-128°.

Cohen, H. *et al, Can. J. Chem.*, 1974, **52**, 66 (*di-Me ester, deriv, ir, pmr*)
Khomitov, R.M. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1978, 1391; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1978, 1210 (*esters, ir, pmr*)
Zoń, J., *Synthesis*, 1984, 661 (*synth, ir, pmr*)

8-Phenyladenosine P-1-00042

[73340-78-0]



$C_{16}H_{17}N_5O_4$ M 343.3

Hygroscopic solid (as hemihydrate).

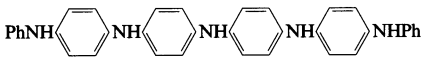
Côngg-Danh, N. *et al*, *Tet. Lett.*, 1979, 3159 (*synth, pmr, cmr*)

Verlinde, C.L.M.J. *et al*, *J. Med. Chem.*, 1994, **37**, 3605 (*synth, uv, pmr, cmr, ms*)

N-[4-(Phenylamino)phenyl]-*N*^{1}-[4-[[4-(phenylamino)phenyl]amino]phenyl]-1,4-benzenediamine, 9CI P-1-00043

N-*Phenylpentaaniline*

[75145-32-3]

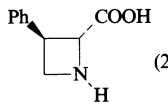


$C_{36}H_{31}N_5$ M 533.6

Microscopic silver-white cryst. Mp 280-281°.

Ochi, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1994, **67**, 1749.

3-Phenyl-2-azetidinecarboxylic acid, 9CI P-1-00044



(2*RS*,3*RS*)-*form*

$C_{10}H_{11}NO_2$ M 177.2

(2RS,3RS)-form

(±)-trans-*form*

Hydrochloride: [158980-44-0]. Solid. Mp 193-194°.

tert-*Butyl ester:* [158980-52-0]. $C_{14}H_{19}NO_2$ M 233.3 Solid (as hydrochloride). Mp 146-148°.

(2RS,3SR)-form

(±)-cis-*form*

Hydrochloride: [158980-45-1]. Solid. Mp 224-226°.

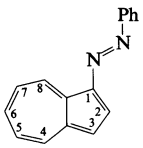
tert-*Butyl ester:* [158980-53-1]. Solid (as hydrochloride). Mp 149-151°.

Blythin, D.J. *et al*, *J.O.C.*, 1994, **59**, 6098 (*synth, pmr*)

1-(Phenylazo)azulene P-1-00045

1-Azulenylphenyldiazene, 9CI. Azulene-1-azobenzene, 8CI

[7206-62-4]



$C_{16}H_{12}N_2$ M 232.2

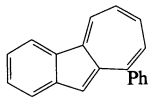
(E)-form

Brown needles (hexane). Mp 121°.

Anderson, A.G. *et al*, *J.A.C.S.*, 1953, **75**, 4980 (*synth*)

Briquet, A.A.S. *et al*, *Helv. Chim. Acta*, 1994, **77**, 1577 (*synth, uv, ir, pmr*)

9-Phenylbenz[*a*]azulene P-1-00046

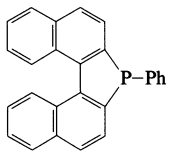


$C_{20}H_{14}$ M 254.3

Dark blue needles. Mp 91.5-92.5°.

Sperandio, D. *et al*, *Helv. Chim. Acta*, 1995, **78**, 765 (*synth, ir, uv, pmr, cmr*)

7-Phenyl-7*H*-benzo[*e*]naphtho[2,1-*b*]phosphindole, 9CI P-1-00047



$C_{26}H_{17}P$ M 360.3

Monodentate ligand with helical chirality. Undergoes spont. resoln. during cryst.

(R)-form

Pale yellow cryst (EtOH). Mp 157.5-159°.

Methiodide: [156747-88-5]. *7-Methyl-7-phenylbenzo*[e]*naphtho*[*2,1*-b]*phosphindolium iodide* $C_{27}H_{20}IP$ M 502.3 Cryst. (CH_2Cl_2/Et_2O). Mp 191-195°.

Ethiodide: [156747-89-6]. *7-Ethyl-7-phenylbenzo*[e]*naphtho*[*2,1*-b]*phosphindolium iodide* $C_{28}H_{22}IP$ M 516.3 Cryst. (CH_2Cl_2/Et_2O). Mp 187-189°.

(±)-form [149639-52-1]

Solid. Mp 157-158° (this may be that of the (*R*)-form).

7-Oxide: [156633-49-7]. $C_{26}H_{17}OP$ M 376.3 Yellow cryst. (EtOAc). Mp 263-264° (may be of the resolved form).

[156854-50-1]

Dore, A. *et al*, *Chem. Comm.*, 1993, 1124 (*synth, ms, pmr, P-31 nmr*)

Watson, A.A. *et al*, *J. Organomet. Chem.*, 1993, **445**, 71 (*synth, pmr*)

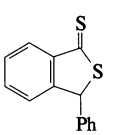
Tani, K. *et al*, *Acta Cryst. C*, 1994, **50**, 769 (*cryst struct*)

Tani, K. *et al*, *J. Organomet. Chem.*, 1994, **469**, 229 (*oxide, ir, uv, pmr, cmr, complexes*)

Gladiali, S. *et al*, *J. Organomet. Chem.*, 1994, **475**, 307 (*complexes*)

Fabbri, D. *et al*, *Synth. Commun.*, 1994, **24**, 1271 (*derivs, ms, pmr, cmr*)

3-Phenylbenzo[*c*]thiophene-1(3*H*)-thione P-1-00048



$C_{14}H_{10}S_2$ M 242.3

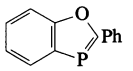
(±)-form

Cryst. Mp 93-94°.

Nishio, T., *J.C.S. Perkin 1*, 1995, 561 (*synth, ir, pmr, cmr*)

2-Phenyl-1,3-benzoxaphosphole P-1-00049

[105865-34-7]



$C_{13}H_9OP$ M 212.1

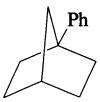
Liq. $Bp_{0.07}$ 124-126°.

Heinicke, J. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1985, **25**, 345 (*synth, ms, uv, cmr, P-31 nmr*)

1-Phenylbicyclo[2.2.1]heptane, 9CI P-1-00050

1-Phenylnorbornane

[24892-79-3]



$C_{13}H_{16}$ M 172.2

Light yellow oil. Bp_{16} 124-128°, Bp_6 65-70°.

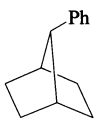
Kleinfilter, D.C. *et al*, *J.O.C.*, 1961, **26**, 3740 (*synth, pmr*)

Olah, G.A. *et al*, *J.A.C.S.*, 1993, **115**, 10728 (*synth, pmr, cmr, ms*)

7-Phenylbicyclo[2.2.1]heptane P-1-00051

7-Phenylnorbornane

[24892-78-2]



$C_{13}H_{16}$ M 172.2

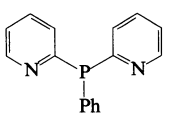
Liq. Bp_2 90-92°.

Olah, G.A. *et al*, *J.O.C.*, 1994, **59**, 2590 (*synth, pmr, cmr, ms*)

Phenylbis(2-pyridinyl)phosphine P-1-00052

2,2′-(Phenylphosphinidene)bispyridine

[68469-71-6]



$C_{16}H_{13}N_2P$ M 264.2

Ligand for Mo, Ru, Os, Pd. Cryst. (EtOH/petrol). Mp 96°. $Bp_{0.1}$ 160°.

Dihydrochloride: Solid. Mp 185-187° sinters at 100°.

Monomethiodide: $C_{17}H_{16}IN_2P$ M 406.2 Solid. Mp 134-135°.

P-*Oxide:* [68469-77-2]. *2,2′-(Phenylphosphinylidene)bispyridine* $C_{16}H_{13}N_2OP$ M 280.2 Solid. Mp 154-155°.

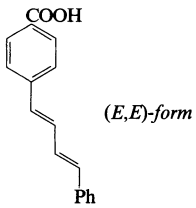
P-*Sulfide: 2,2′-(Phenylphosphinothioylidene) bispyridine* $C_{16}H_{13}N_2PS$ M 296.3 Cryst. (EtOH). Mp 141°.

P-*Sulfide, dihydrochloride:* Solid. Mp 165-171°.

Mann, F.G. *et al*, *J.O.C.*, 1948, **13**, 502 (*synth, derivs*)
Schmidbaur, H. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1329 (*synth, pmr, cmr, P-31 nmr*)
Newkome, G.R. *et al*, *Inorg. Chem.*, 1987, **26**, 3500 (*complexes*)
Uchida, Y. *et al*, *Heteroat. Chem.*, 1990, **1**, 295 (*synth, oxide*)
Espinet, P. *et al*, *J. Organomet. Chem.*, 1993, **450**, 145 (*complexes*)
Deeming, A.J. *et al*, *J.C.S. Dalton*, 1993, 2041, 3383 (*complexes*)

4-(4-Phenyl-1,3-butadienyl) benzoic acid, 9CI P-1-00053

[62589-83-7]



(*E,E*)-*form*

$C_{17}H_{14}O_2$ M 250.2

(E,E)-form
Needles (Me_2CO). Mp 230-265°.

Me ester: [89510-60-1].
$C_{18}H_{16}O_2$ M 264.3 Cryst. (C_6H_6/cyclohexane). Mp 180-180.5° (164-168°).

Et ester: [163276-32-2].
$C_{19}H_{18}O_2$ M 278.3 Retinoid. Yellow cryst. (hexane/EtOAc). Mp 120-121°.

Nitrile: [37985-14-1]. *4-(4-Phenyl-1,3-butadienyl)benzonitrile*
$C_{17}H_{13}N$ M 231.2 Cryst. (MeOH). Mp 163-164°.

[1552-40-5, 101723-02-8]

McDonald, R.N. *et al*, *J.O.C.*, 1959, **24**, 1969 (*Me ester*)
Zweig, A. *et al*, *J.A.C.S.*, 1967, **89**, 4091 (*nitrile*)
Quina, F.H. *et al*, *Z. Phys. Chem.*, 1976, **101**, 151 (*synth*)
Gaudiana, R.A. *et al*, *J. Polym. Sci., Polym. Chem. Ed.*, 1987, **25**, 1249 (*Me ester*)
Torrado, A. *et al*, *Synthesis*, 1995, 285 (*Et ester*)

1-Phenyl-1,2-butanedione, 9CI P-1-00054

Ethyl phenyl diketone

[3457-55-4]

$PhCOCOCH_2CH_3$

$C_{10}H_{10}O_2$ M 162.1
Yellow liq. Bp_{20} 130-132°, $Bp_{0.5}$ 74-76°. n_D^{19} 1.5239.

2-Oxime: [25994-02-9].
$C_{10}H_{11}NO_2$ M 177.2 Mp 116-119°.

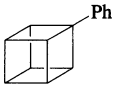
Dioxime:
$C_{10}H_{12}N_2O_2$ M 192.2 Mp 205-206°.

Coles, H.W. *et al*, *J.A.C.S.*, 1929, **51**, 2269 (*synth*)
Lynn, J.W. *et al*, *J.A.C.S.*, 1951, **73**, 4284 (*synth*)
Emmons, W.D. *et al*, *J.A.C.S.*, 1955, **77**, 4415 (*synth*)
Torii, S. *et al*, *Synthesis*, 1987, 377 (*synth, ir, pmr*)
Page, P.C.B. *et al*, *Tetrahedron*, 1992, **48**, 7265 (*synth, ir, pmr*)
Murakami, M. *et al*, *Synlett*, 1993, 511 (*synth, pmr, cmr*)
Page, P.C.B. *et al*, *Synthesis*, 1995, 73 (*synth, ir, pmr*)

Phenylcubane P-1-00055

Phenylpentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane, 9CI

[132657-48-8]

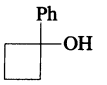


$C_{14}H_{12}$ M 180.2
Oil.

Olah, G.A. *et al*, *J.A.C.S.*, 1993, **115**, 10728 (*synth, pmr, cmr, ms*)

1-Phenylcyclobutanol, 9CI P-1-00056

[935-64-8]



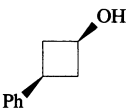
$C_{10}H_{12}O$ M 148.2
Liq. $Bp_{0.05}$ 40-42°.

4-Nitrobenzoyl: [29586-27-4].
Solid (heptane). Mp 97-99°.

3,5-Dinitrobenzoyl: [18592-80-8].
Cryst. (petrol/C_6H_6 3:1). Mp 107-108°.

Roberts, D.D., *J.O.C.*, 1969, **34**, 285 (*deriv, pmr*)
Padwa, A. *et al*, *J.A.C.S.*, 1970, **92**, 5674 (*deriv, ir, ms*)
Chochua, K.A. *et al*, *Zh. Org. Khim.*, 1972, **8**, 1867; *J. Org. Chem. USSR (Engl. Transl.)*, 1972, **8**, 1914 (*ms*)
Finkelshtein, E.S., *Neftekhimiya*, 1980, **20**, 75; *CA*, **93**, 26003y (*synth*)
Pritzkow, W. *et al*, *J. Prakt. Chem.*, 1989, **331**, 424; 1990, **332**, 381 (*synth, cmr*)
Çelebi, S. *et al*, *J.A.C.S.*, 1993, **115**, 8613 (*synth, ir, pmr*)

3-Phenylcyclobutanol, 9CI P-1-00057



$C_{10}H_{12}O$ M 148.2

(1RS,3SR)-form [150639-15-9]
cis-*form*
Liq. $Bp_{0.6}$ 90-95° ($Bp_{<1}$ 62-64°).

4-Methylbenzenesulfonyl: [26505-63-5].
Oil.

4-Nitrobenzoyl: Long needles (EtOAc/hexane). Mp 131.1-131.6°.

[26505-64-6, 150639-16-0]

Manatt, S.L. *et al*, *J.A.C.S.*, 1964, **86**, 2645 (*synth, ir*)
Wiberg, K.B. *et al*, *J.A.C.S.*, 1993, **115**, 10645 (*synth*)

1-Phenylcyclobutene P-1-00058

1-Cyclobuten-1-ylbenzene, 9CI

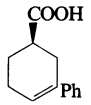
[3365-26-2]

$C_{10}H_{10}$ M 130.1
Pale yellow oil. $Bp_{3.5}$ 74-75°, $Bp_{0.01}$ 37°. n_D^{25} 1.5639.

Berger, A. *et al*, *J. Med. Chem.*, 1960, **2**, 687 (*synth*)
Mant, G.R. *et al*, *J.C.S. Faraday 2*, 1981, **77**, 1487 (*uv*)
Dass, C. *et al*, *Org. Mass Spectrom.*, 1983, **18**, 542 (*ms*)
Hohlneicher, G. *et al*, *J.A.C.S.*, 1988, **110**, 4483 (*struct, pe*)
Trace, R.L. *et al*, *J. Organomet. Chem.*, 1989, **376**, 103 (*cmr*)
Çelebi, S. *et al*, *J.A.C.S.*, 1993, **115**, 8613 (*synth, ms*)

3-Phenyl-3-cyclohexene-1-carboxylic acid, 9CI P-1-00059

2,3,4,5-Tetrahydro-3-biphenylcarboxylic acid



(*R*)-*form*

$C_{13}H_{14}O_2$ M 202.2

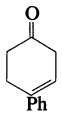
(R)-form [150013-81-3]
Powder. Mp 74-76.5°. $[\alpha]_D^{24}$ +28.4 (c, 1.14 in $CHCl_3$) (97% ee).

(±)-form
Solid. Mp 111-112°.

Wright, J.L. *et al*, *J. Med. Chem.*, 1994, **37**, 3523 (*synth, pmr, resoln, cmr, ms*)

4-Phenyl-3-cyclohexen-1-one P-1-00060

[51171-71-2]



$C_{12}H_{12}O$ M 172.2
Cryst. (petrol). Mp 47-48°, Mp 72-73° (62-63°). Cryst. slowly liquefy on standing.

Oxime: [51171-76-7].
$C_{12}H_{13}NO$ M 187.2 Cryst. (hexane). Mp 93-94°.

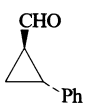
2,4-Dinitrophenylhydrazone: [51171-74-5].
Yellow-brown cryst. (butanol). Mp 168-170° (145-146°).

Bergmann, E.D. *et al*, *J.A.C.S.*, 1959, **81**, 2772 (*synth, uv*)
Carenini, G. *et al*, *Farmaco, Ed. Sci.*, 1973, **28**, 896 (*synth, oxime*)
Duhamel, P. *et al*, *Tetrahedron*, 1986, **42**, 4777 (*pmr, cmr, ir*)
Cory, R.M. *et al*, *Synth. Commun.*, 1994, **24**, 799 (*synth, pmr, cmr, ms*)

2-Phenylcyclopropane-carboxaldehyde P-1-00061

1-Formyl-2-phenylcyclopropane

[67074-44-6]



(1*RS*,2*RS*)-*form*

$C_{10}H_{10}O$ M 146.1

(1RS,2RS)-form [34271-31-3]
(±)-trans-*form*
Oil. Bp_5 93-95°. Readily oxidised by air.

(1RS,2SR)-form [34271-30-2]

(±)-cis-*form*
Oil. Bp_5 100°.

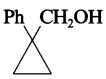
[79929-84-3, 82263-48-7, 82263-50-1]

Levina, R.Ya. *et al, J. Org. Chem. USSR (Engl. Transl.)*, 1977, **13**, 58 (*synth*)
Baldwin, J. *et al, J.A.C.S.*, 1984, **106**, 1421 (*synth, ir, pmr*)
Abdallah, H. *et al, Bull. Soc. Chim. Fr.*, 1985, 794 (*synth, ir, pmr*)
Alonso, M.E. *et al, Magn. Reson. Chem.*, 1991, **28**, 956 (*ir, pmr, cmr*)
Zelechonek, Y. *et al, J.O.C.*, 1992, **57**, 5785, 5787 (*synth, pmr*)

1-Phenylcyclopropanemethanol P-1-00062

1-Hydroxymethyl-1-phenylcyclopropane

[31729-66-5]



$C_{10}H_{12}O$ M 148.2
Liq. Bp_{112} 117-122°.

Lowger, P. *et al, Helv. Chim. Acta*, 1959, **42**, 2394 (*synth*)
Wilt, J.W. *et al, J.O.C.*, 1962, **27**, 3430 (*synth*)
Hutton, H.M. *et al, Can. J. Chem.*, 1963, **41**, 2429 (*pmr*)
Harrison, I.T. *et al, J.O.C.*, 1971, **36**, 3515 (*synth*)

1-Phenylcyclopropylamine P-1-00063

1-Phenylcyclopropanamine, 9CI

[41049-53-0]

$C_9H_{11}N$ M 133.1

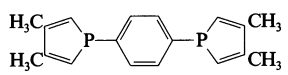
Hydrochloride: [73930-39-9].
Cryst. Mp 198-198.5°.

Bunce, S.C. *et al, J.A.C.S.*, 1954, **76**, 2244 (*synth*)
Warren, J.D. *et al, Synth. Commun.*, 1980, **10**, 107 (*synth*)
De Boer, J.S.A.M. *et al, Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1990, **109**, 375 (*cryst struct*)

1,4-Phenylenebis(3,4-dimethyl-1*H*-phosphole) P-1-00064

1,1'-(1,4-Phenylene)bis[3,4-dimethyl-1H-phosphole], 9CI. 1,4-Bis(3,4-dimethyl-1H-phospholyl)benzene

[130653-03-1]



$C_{18}H_{20}P_2$ M 298.3
Cryst. (CH_2Cl_2/hexane). Mp 162°.

Mercier, F. *et al, Heteroat. Chem.*, 1990, **1**, 187 (*synth, pmr, cmr, P-31 nmr*)

1,4-Phenylenebis [phenyliodonium], 9CI P-1-00065

$C_{18}H_{14}I_2^{2\oplus}$ M 484.1 (ion)

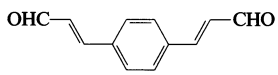
Bis(trifluoromethanesulfonate): [138996-14-2].
$C_{20}H_{14}F_6I_2O_6S_2$ M 782.2 Microcryst. Mp 280-190° dec.

Kitamura, T. *et al, Mendeleev Commun.*, 1991, 148 (*synth, pmr, cmr*)
Gallop, P.M. *et al, J.A.C.S.*, 1993, **115**, 11702 (*synth*)

3,3'-(1,4-Phenylene)bis-2-propenal, 9CI P-1-00066

1,4-Phenylenediacylaldehyde. β,β-p-Phenylenediacrolein

[3049-37-4]



$C_{12}H_{10}O_2$ M 186.2

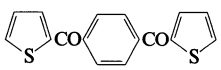
(E,E)-form [63405-68-5]
Cryst. Mp 159-162°.

Lüttringhaus, A. *et al, Chem. Ber.*, 1960, **93**, 3048 (*synth, uv*)
Sonoda, Y. *et al, J.C.S. Perkin 1*, 1993, 1147 (*synth, ir, pmr*)

1,2-Phenylenebis[2-thienylmethanone], 9CI P-1-00067

1,4-Di(2-thenoyl)benzene

[146474-88-6]



$C_{16}H_{10}O_2S_2$ M 298.3
Pale yellow needles (xylene). Mp 227°.

Ohta, A. *et al, J.C.S. Perkin 1*, 1993, 905 (*synth, ir, pmr, ms*)

1-Phenylethanethione P-1-00068

Phenyl methyl thioketone. Thioacetophenone

[16696-68-7]

$PhC(S)CH_3$

C_8H_8S M 136.2
Bp_{12} 97-100°. n_D^{20} 1.64.

Sammes, M.P. *et al, J.C.S. Perkin 1*, 1991, 183.
Capperucci, A. *et al, J.O.C.*, 1991, **56**, 7323 (*synth*)

2-Phenyl-1,1,1-ethanetricarboxylic acid P-1-00069

$PhCH_2C(COOH)_3$

$C_{11}H_{10}O_6$ M 238.1

Tri-Et ester: [16515-84-7].
$C_{17}H_{22}O_6$ M 322.3 Liq. Bp_{12} 195-197°.

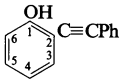
Trinitrile: [6023-46-7]. *1,1,1-Tricyano-2-phenylethane. 2,2-Dicyano-3-phenylpropionitrile. Benzylcyanoform*
$C_{11}H_7N_3$ M 181.1 Yellowish needles ($CHCl_3$); cryst. (1,2-dichloroethane/petrol). Mp 138°. Sublimes.

Hantzsch, A. *et al, Ber.*, 1899, **32**, 641 (*trinitrile, synth*)
Sheppard, W.A. *et al, J.O.C.*, 1966, **31**, 919 (*trinitrile, synth*)
Prelicz, D. *et al, Pol. J. Chem. (Rocz. Chem.)*, 1967, **41**, 267 (*tri-Et ester, synth*)
Rüchardt, C. *et al, Chem. Ber.*, 1994, **127**, 2225 (*trinitrile, synth, pmr, cmr, ms, ir*)

2-(Phenylethynyl)phenol, 9CI P-1-00070

2-Hydroxytolan. o-Hydroxydiphenylacetylene. (2-Hydroxyphenyl)phenylacetylene

[92151-73-0]



$C_{14}H_{10}O$ M 194.2
Cryst. Mp 69-70°. Bp_6 180°.

Me ether: [41398-67-8]. *1-Methoxy-2-(phenylethynyl)benzene, 9CI. o-(Phenylethynyl)anisole, 8CI. 2-Methoxytolan*
$C_{15}H_{12}O$ M 208.2 Oil. Bp_1 172-173°.

Letsinger, R.L. *et al, J.O.C.*, 1961, **26**, 1271 (*synth, uv, ir*)
Buckle, D.R. *et al, J.C.S. Perkin 1*, 1985, 2443 (*Me ether*)
Sagi, M. *et al, Heterocycles*, 1990, **30**, 1009 (*synth*)
Kondo, Y. *et al, Tetrahedron*, 1994, **59**, 11803 (*synth, pmr*)

3-(Phenylethynyl)phenol, 9CI P-1-00071

3-Hydroxytolan. m-Hydroxydiphenylacetylene. (3-Hydroxyphenyl)phenylacetylene

[111731-38-5]

$C_{14}H_{10}O$ M 194.2
Endcapper for arylene polymers. Needles (hexane). Mp 86°.

Ac: [153614-82-5].
$C_{16}H_{12}O_2$ M 236.2 Mp 53-54°.

Me ether: 1-Methoxy-3-(phenylethynyl)benzene, 9CI. m-(Phenylethynyl)anisole, 9CI. 3-Methoxytolan
$C_{15}H_{12}O$ M 208.2 Prisms. Mp 74-76°.

Chen, Q.-Y. *et al, Synthesis*, 1988, 897 (*Me ether*)
Jayaraman, S. *et al, Polym. Prepr., (Am. Chem. Soc., Div. Polym. Chem.)*, 1993, **34**, 511 (*synth, Ac, ir, pmr*)
Mataka, S. *et al, Synthesis*, 1995, 133 (*Me ether*)

4-(Phenylethynyl)phenol, 9CI P-1-00072

4-Hydroxytolan. p-Hydroxydiphenylacetylene. (4-Hydroxyphenyl)phenylacetylene

[1849-26-9]

$C_{14}H_{10}O$ M 194.2
Needles (petrol). Mp 83-84°, Mp 123-125°.

Me ether: [7380-78-1]. *1-Methoxy-4-(phenylethynyl)benzene, 9CI. p-(Phenylethynyl)anisole, 8CI. 4-Methoxytolan*
$C_{15}H_{12}O$ M 208.2 Plates (MeOH). Mp 58-59°.

Ph ether: [92566-01-3]. *1-Phenoxy-4-(phenylethynyl)benzene, 9CI. 4-Phenoxytolan*
$C_{20}H_{14}O$ M 270.3 Plates. Mp 77-78°.

Katritzky, A.R. *et al, J.C.S.*, 1960, 1519 (*Me ether*)
Stephens, R.D. *et al, J.O.C.*, 1963, **28**, 3313 (*synth, Me ether*)
Gorshkova, G.N. *et al, Zh. Fiz. Khim.*, 1964, **38**, 2485; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1344 (*uv, ir*)
McEwen, W.E. *et al, J. Fluorine Chem.*, 1984, **25**, 169 (*Me ether, Ph ether*)
Swiss, K.A. *et al, Synthesis*, 1992, 127 (*synth, ir*)

1-Phenyl-1,3-hexanediol P-1-00073

$PhCH(OH)CH_2CH(OH)CH_2CH_2CH_3$

$C_{12}H_{18}O_2$ M 194.2

(±)-*form*
Bp_{11} 170-172°.

1-Ac:
$C_{14}H_{20}O_3$ M 236.3 Bp_{11} 179-181°.

Emerson, W.S., *J.O.C.*, 1945, **10**, 464 (*synth, 1-Ac*)
Behrens, K. *et al*, *Annalen*, 1995, 385 (*synth, pmr, ir*)

1-Phenyl-1,6-hexanediol, 9CI P-1-00074

[4066-82-4]

$PhCH(OH)(CH_2)_4CH_2OH$

$C_{12}H_{18}O_2$ M 194.2

(±)-*form*
Cryst. (hexane/Et_2O). Mp 57-58°. $Bp_{0.02}$ 135-139°.

Di-Ac: [103187-14-0].
$C_{16}H_{22}O_4$ M 278.3 Oil.

Kwart, H. *et al*, *J.A.C.S.*, 1959, **81**, 943 (*synth*)
Mornet, R. *et al*, *Bull. Soc. Chim. Fr.*, 1965, 3043 (*synth*)
Eur. Pat., 171 251, (1986); *CA*, **105**, 42484c (*di-Ac*)

4-Phenyl-1*H*-indole, 9CI P-1-00075

[35577-92-5]

$C_{14}H_{11}N$ M 193.2
Cryst. Mp 58-60°, Mp 76-77°.

Muratake, H. *et al*, *Heterocycles*, 1990, **31**, 691 (*synth, pmr*)
Andrews, J.F.P. *et al*, *Tetrahedron*, 1993, **49**, 7353 (*synth, ir, pmr, cmr*)

5-Phenyl-1*H*-indole, 9CI P-1-00076

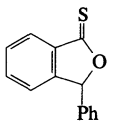
[66616-72-6]

$C_{14}H_{11}N$ M 193.2
Cryst. Mp 71-73°.

Yang, Y. *et al*, *J. Het. Chem.*, 1992, **34**, 1169, 1395 (*synth*)

3-Phenyl-1(3*H*)-isobenzofuranthione, 9CI P-1-00077

[163226-46-8]



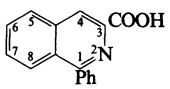
$C_{14}H_{10}OS$ M 226.2

(±)-*form*
Fine yellow plates. Mp 97-99°.

Nishio, T., *J.C.S. Perkin 1*, 1995, 561 (*synth, ir, pmr, cmr*)
Bailey, J.H. *et al*, *J.C.S. Perkin 1*, 1995, 589 (*synth, pmr, cmr, ir*)

1-Phenyl-3-isoquinolinecarboxylic acid P-1-00078

[66528-01-6]



$C_{16}H_{11}NO_2$ M 249.2
Yellow needles (MeCN). Mp 222-223°.

Et ester: [81803-40-9].
$C_{18}H_{15}NO_2$ M 277.3 Cryst. (petrol). Mp 100-101°.

Filler, R. *et al*, *J.O.C.*, 1962, **27**, 2403 (*synth*)
Walsh, D.A. *et al*, *J. Med. Chem.*, 1978, **21**, 583 (*synth*)
Hickey, D.M.B. *et al*, *J.C.S. Perkin 1*, 1984, 2189; 1987, 921 (*Et ester*)

1-Phenyl-4-isoquinolinecarboxylic acid P-1-00079

[90829-28-0]

$C_{16}H_{11}NO_2$ M 249.2
Mp 244-247° (215-217°).

Nitrile: [41969-01-1]. *4-Cyano-1-phenylisoquinoline*
$C_{16}H_{10}N_2$ M 230.2 Pale orange needles (C_6H_6/petrol). Mp 142°.

Ger. Pat., 3 233 424, (1984); *CA*, **101**, 38362m (*synth, nitrile*)
Bartmann, W. *et al*, *Heterocycles*, 1989, **29**, 707 (*synth, pmr*)

3-Phenyl-4-isoquinolinecarboxylic acid P-1-00080

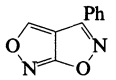
$C_{16}H_{11}NO_2$ M 249.2

Et ester: [109802-64-4].
$C_{18}H_{15}NO_2$ M 277.3 Oil.

Nitrile: 4-Cyano-3-phenylisoquinoline
$C_{16}H_{10}N_2$ M 230.2 Yellow needles. Mp 155-157°.

Maassarani, F. *et al*, *Organometallics*, 1987, **6**, 2029 (*Et ester*)
Suzuki, H. *et al*, *Synthesis*, 1995, 763 (*nitrile*)

3-Phenylisoxazolo[5,4-*c*]isoxazole P-1-00081



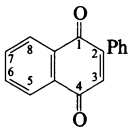
$C_{10}H_6N_2O_2$ M 186.1
Yellow prisms (MeOH). Mp 146-147°.

Anderson, D.J. *et al*, *J. Het. Chem.*, 1995, **32**, 1189.

2-Phenyl-1,4-naphthoquinone P-1-00082

2-Phenyl-1,4-naphthalenedione, 9CI

[2348-77-8]



$C_{16}H_{10}O_2$ M 234.2
Yellow cryst. Mp 111-112°.

Courseille, C. *et al*, *C. R. Hebd. Seances Acad. Sci. Ser. C*, 1969, **268**, 1358 (*cryst struct*)
Singh, P.K. *et al*, *Synth. Commun.*, 1992, **22**, 987 (*synth, ir, pmr*)
Harrity, J.P.A. *et al*, *Tetrahedron*, 1993, **49**, 5565 (*synth, ir, pmr*)

5-Phenyl-1,4-naphthoquinone P-1-00083

5-Phenyl-1,4-naphthalenedione, 9CI

[33522-29-1]

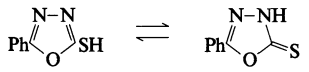
$C_{16}H_{10}O_2$ M 234.2
Orange plates (MeOH). Mp 169.5-170°.

House, H.O. *et al*, *J.O.C.*, 1972, **37**, 1003 (*synth, ir, uv, pmr, ms*)

5-Phenyl-1,3,4-oxadiazole-2-thiol P-1-00084

5-Phenyl-1,3,4-oxadiazole-2(3H)-thione, 9CI. 2-Mercapto-5-phenyl-1,3,4-oxadiazole. 2-Phenyl-Δ²-1,3,4-oxadiazoline-5-thione

[3004-42-0]

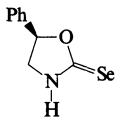


$C_8H_6N_2OS$ M 178.2
NH-form predominates. Cryst. (MeOH). Mp 219-220°. pK_a 5.25.

▶ Irritant. Air-sensitive.

Hogarth, E. *et al*, *J.C.S.*, 1952, 4811 (*synth*)
Young, R.W. *et al*, *J.A.C.S.*, 1955, **77**, 400 (*synth*)
Chau, N. *et al*, *J. Het. Chem.*, 1982, **19**, 541 (*synth*)
Aranda, G. *et al*, *Org. Magn. Reson.*, 1982, **18**, 159 (*cmr*)
Shawali, A.S. *et al*, *Heterocycles*, 1983, **20**, 2211 (*tautom*)
Charistos, D.A. *et al*, *J. Het. Chem.*, 1994, **31**, 1593 (*uv, ir, tautom*)

4-Phenyl-2-oxazolidineselone, 9CI P-1-00085



C_9H_9NOSe M 226.1

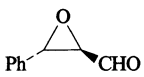
(*R*)-*form* [136794-56-4]
Cryst. Mp 134-137°. $[\alpha]_D$ −53 (c, 0.64 in $CHCl_3$).

Peng, J. *et al*, *J.O.C.*, 1994, **59**, 4977 (*synth, uv, ir, pmr, cmr, Se-77 nmr*)

3-Phenyloxiranecarboxaldehyde, 9CI P-1-00086

β-Phenylglycidaldehyde. 2,3-Epoxycinnamaldehyde

[5693-99-2]



(2*R*,3*S*)-*form*

$C_9H_8O_2$ M 148.1

(2*R*,3*S*)-*form* [126720-47-6]
(2R-trans)-*form*
$[\alpha]_D^{25}$ +86 (c, 2.1 in $CHCl_3$) (>95% ee).

(±)-*form*
Liq. $Bp_{0.2}$ 66-68°. Isomeric composition not specified.

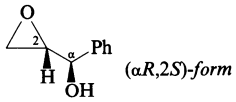
[71403-94-6, 119951-98-3, 119951-99-4, 121651-02-3]

Payne, G.B., *J.O.C.*, 1960, **25**, 275; 1961, **26**, 250 (*synth*)

Arbuzov, B.A. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1979, 1257; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1979, 1173 (*ir, pmr, props*)
Miyashita, M. *et al*, *Chem. Lett.*, 1987, **2**, 285 (*synth*)
Hu, Y. *et al*, *Synth. Commun.*, 1988, **18**, 1607 (*synth*)
Evans, D.L. *et al*, *Tet. Lett.*, 1988, **29**, 5065 (*synth*)
Yu, L. *et al*, *Chem. Comm.*, 1993, 232 (*synth*)

α-Phenyloxiranemethanol, 9CI P-1-00087

2,3-Epoxy-1-phenyl-1-propanol



(α*R*,2*S*)-*form*

$C_9H_{10}O_2$ M 150.1

(α*R*,2*S*)-*form* [107643-29-8]
$[\alpha]_D^{23}$ −100.2 (c, 2.31 in $CHCl_3$).

(α*S*,2*S*)-*form* [107643-32-3]
Oil. $[\alpha]_D^{23}$ +87.5 (c, 2.3 in $CHCl_3$).

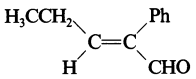
[127913-26-2, 127913-27-3, 153062-14-7, 153062-15-8]

Palazón, J.M. *et al*, *Tet. Lett.*, 1986, **27**, 4987 (*synth*)
Kawakani, T. *et al*, *J.O.C.*, 1993, **58**, 7608 (*synth, ir, pmr*)
Dittmer, D.C. *et al*, *J.O.C.*, 1994, **59**, 1004 (*synth, pmr*)

2-Phenyl-2-pentenal P-1-00088

α-*Propylidenebenzeneacetaldehyde, 9CI*

[3491-63-2]



$C_{11}H_{12}O$ M 160.2

(*E*)-*form* [42762-46-9]
$Bp_{0.1}$ 62°.
▶ Irritant.

Bouget, H., *Bull. Soc. Chim. Fr.*, 1965, 2063 (*synth, uv, ir*)
Dana, G. *et al*, *Bull. Soc. Chim. Fr.*, 1973, 1676 (*synth, pmr, uv, ir*)

2-Phenyl-4-pentynoic acid P-1-00089

Phenylpropargylacetic acid

$HC{\equiv}CCH_2CHPhCOOH$

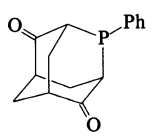
$C_{11}H_{10}O_2$ M 174.1

(±)-*form*
Mp 96-97°.

Vincent, M. *et al*, *Bull. Soc. Chim. Fr.*, 1962, 1580.
Bell, I.M. *et al*, *J.C.S. Perkin 1*, 1994, 1997 (*synth*)

2-Phenyl-2-phosphatricyclo[3.3.1.1^{3,7}]decan-4,8-dione P-1-00090

[122557-75-9]



(−)-*form*

$C_{15}H_{15}O_2P$ M 258.2

(−)-*form* [126456-50-6]
Cryst. (propan-2-ol). Mp 142-144°. $[\alpha]_D^{25}$ −674 ($CHCl_3$).

Methiodide: [126456-52-8]. *2-Methyl-4,8-dioxo-2-phenyl-2-phosphoniatricyclo[3.3.1.1^{3,7}]decane*
$C_{16}H_{18}IO_2P$ M 400.1 Cryst. ($MeNO_2$). Mp 260-262°. $[\alpha]_D^{25}$ −29.9 (MeOH).

2-Oxide: [126456-51-7].
$C_{15}H_{15}O_3P$ M 274.2 Cryst. (propan-2-ol). Mp 210-212°.

(±)-*form* [126412-53-1]

Methiodide: [126412-52-0].
Solid. Mp 260-262°.

2-Oxide: [89784-09-8].
Solid. Mp 186-188°.

Zemlyanoi, V.N. *et al*, *Zh. Obshch. Khim.*, 1989, **59**, 476, 1451; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1989, **59**, 423, 1290 (*synth, ir, ms, pmr, cmr, P-31 nmr*)

1-Phenylphosphetane, 9CI P-1-00091

[142599-70-0]

$C_9H_{11}P$ M 150.1
Ligand for Mo and Fe. Oil. $Bp_{0.05}$ 63°. Unstable, polymerises rapidly.

Bader, A. *et al*, *J.C.S. Dalton*, 1992, 1751 (*complex*)
Kang, Y.B. *et al*, *Chem. Comm.*, 1994, 475, 1404 (*synth, pmr, cmr, P-31 nmr, complex*)

Phenylphosphinediacetic acid P-1-00092

2,2′-(Phenylphosphinidene)bisacetic acid

[58942-13-5]

$PhP(CH_2COOH)_2$

$C_{10}H_{11}O_4P$ M 226.1

Di-Me ester: [17166-63-1]. *Dimethyl 2,2′-(phenylphosphinidene)bisacetate*
$C_{12}H_{15}O_4P$ M 254.2 Liq. Bp_1 147-149°, $Bp_{0.4}$ 125°.

Di-Et ester: [38080-06-7]. *Diethyl 2,2′-(phenylphosphinidene)bisacetate*
$C_{14}H_{19}O_4P$ M 282.2 Liq. d_4^{20} 1.14. $Bp_{0.05}$ 122-124°. n_D^{20} 1.5280.

Dinitrile: [61806-56-2]. *Bis(cyanomethyl) phenylphosphine. 2,2′-(Phenylphosphinidene) bisacetonitrile*
$C_{10}H_9N_2P$ M 188.1 Solid. Insol. H_2O; v. sol. $CHCl_3$. Mp 59-62°. $Bp_{0.25}$ 148-150°.

Ismagolov, R.K. *et al*, *Zh. Obshch. Khim.*, 1972, **42**, 1248; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1972, **42**, 1243 (*di-Et ester*)
Dahl, O., *Acta Chem. Scand., Ser. B*, 1976, **30**, 799 (*synth, ir, pmr, P-31 nmr, dinitrile*)
Novikova, Z.S. *et al*, *Zh. Obshch. Khim.*, 1976, **46**, 575; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1976, **46**, 572 (*di-Me ester, synth, ir, P-31 nmr*)
Podlahová, J., *Coll. Czech. Chem. Comm.*, 1978, **43**, 57; 1979, **44**, 2460 (*synth, ir, uv, props, complexes*)
Podlahová, J. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1988, **37**, 87 (*ester, synth, ir, ms, pmr, cmr, P-31 nmr*)

P,P′-[(Phenylphosphinidene) di-2,1-ethanediyl]bis[*N,N,N′,N′*-tetramethylphosphonous diamide] P-1-00093

[63578-28-9]

$PhP[CH_2CH_2P(NMe_2)_2]_2$

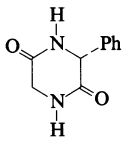
$C_{18}H_{37}N_4P_3$ M 402.4
Ligand. Viscous yellow liq. which slowly cryst. Mp 38-40°. $Bp_{0.005}$ 155-162°.

King, R.B. *et al*, *J.A.C.S.*, 1977, **99**, 4001 (*synth, pmr, cmr, P-31 nmr*)

3-Phenyl-2,5-piperazinedione, 9CI P-1-00094

cyclo-*Glycylphenylglycyl*

[21746-02-1]



(*R*)-*form*

$C_{10}H_{10}N_2O_2$ M 190.2

(*R*)-*form* [81554-02-1]
Cryst. (EtOAc/petrol). Mp 241-243°. $[\alpha]_D^{23}$ −696 (c, 0.05 in DMSO).

(*S*)-*form* [134521-82-7]
Cryst.

(±)-*form*
Cryst. (H_2O). Mp 242-243°.

[156869-21-5]

Kopple, K.D. *et al*, *J.A.C.S.*, 1969, **91**, 962 (*synth, conformn*)
Barfield, M. *et al*, *J.A.C.S.*, 1982, **104**, 3302 (*synth, pmr, ir*)
Sato, N. *et al*, *J. Het. Chem.*, 1986, **23**, 1677 (*synth, pmr, ir, bibl*)
Szkaradzinska, M.B. *et al*, *Acta Cryst. C*, 1994, **50**, 565 (*cryst struct*)

1-Phenyl-2-propyn-1-amine P-1-00095

3-Amino-3-phenylpropyne

$HC{\equiv}CCHPhNH_2$

C_9H_9N M 131.1

(±)-*form*
Cryst. (EtOH) (as hydrochloride).

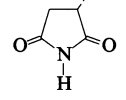
N-*Ac:*
$C_{11}H_{11}NO$ M 173.2 Needles (Et_2O/hexane).

Noro, M. *et al*, *J.A.C.S.*, 1994, **116**, 6179 (*synth, pmr*)

3-Phenyl-2,5-pyrrolidinedione, 9CI P-1-00096

2-Phenylsuccinimide, 8CI

[3464-18-4]



(*R*)-*form*

$C_{10}H_9NO_2$ M 175.1

(*R*)-*form* [114531-20-3]
Mp 83-94° (partial racemate). $[\alpha]_D^{20}$ +151 (c, 2 in EtOH).

(±)-*form*
Mp 90°. Bp_{11} 223-225°. pK_a 8.73 (4% EtOH aq.).

N-*Me:* [86-34-0]. *1-Methyl-3-phenyl-2,5-pyrrolidinedione, 9CI.* N-*Methyl-2-phenylsuccinimide, 8CI.* ***Phensuximide***
$C_{11}H_{11}NO_2$ M 189.2 Antiepileptic drug. Cryst. (EtOH). Mp 69-71°.

[34367-67-4, 54807-40-8, 97233-03-9, 97233-04-0, 114531-21-4]

Miller, C.A. *et al, J.A.C.S.*, 1951, **73**, 4895 (*synth*)
Foucaud, A. *et al, Bull. Soc. Chim. Fr.*, 1965, 2552 (*ir*)
Kornet, M.J. *et al, J. Med. Chem.*, 1977, **20**, 1210 (*synth*)
Wijnberg, J.B.P. *et al, Tetrahedron*, 1978, **34**, 179 (*synth*)
Ferrendelli, J.A. *et al, Adv. Neurol.*, 1980, **27**, 587 (*pharmacol, rev, N-Me*)
Yang, Z.Y. *et al, J. Chromatogr.*, 1985, **324**, 444 (*resoln, hplc, N-Me*)
Polański, T., *J.C.S. Perkin 1*, 1988, 629 (*synth, ir, pmr, cd, R-form*)

(Phenylseleno)acetylene P-1-00097

(*Ethynylseleno*)*benzene, 9CI.* (*Phenylseleno*)*ethyne. Ethynyl phenyl selenide*

[65910-12-5]

PhSeC≡CH

C_8H_6Se M 181.0
Liq. with pungent odour. Bp_{17} 104-105°, $Bp_{0.2}$ 60°.

Chierichi, L. *et al, Gazz. Chim. Ital.*, 1956, **86**, 1269 (*synth*)
Radeglia, R. *et al, J. Organomet. Chem.*, 1987, **327**, 7 (*cmr, Se-77 nmr*)
Braga, A.L. *et al, Synth. Commun.*, 1994, **24**, 1165 (*synth, pmr*)

2-(Phenylseleno)ethylamine P-1-00098

2-(Phenylseleno)ethanamine

[81418-58-8]

$PhSeCH_2CH_2NH_2$

$C_8H_{11}NSe$ M 200.1
Yellow liq. $Bp_{0.15}$ 74-78°.

Exon, C. *et al, J.A.C.S.*, 1983, **105**, 4739 (*synth, pmr, ir*)
Billimoria, A.D. *et al, J.O.C.*, 1994, **59**, 6777 (*synth, pmr*)

(Phenylseleno)ethylene P-1-00099

(*Ethenylseleno*)*benzene, 9CI. Phenyl vinyl selenide*

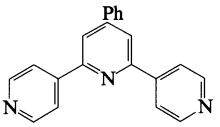
[35167-28-3]

$PhSeCH{=}CH_2$

C_8H_8Se M 183.1
Oil. Bp_5 63-65°.

Kushnarev, D.F. *et al, Zh. Org. Khim.*, 1976, **12**, 1482; 1990, **26**, 19; *J. Org. Chem. USSR* (*Engl. Transl.*), 1976, **12**, 1465; 1990, **26**, 15 (*cmr, pmr, Se-77 nmr*)
Reich, H.J. *et al, J.O.C.*, 1981, **46**, 2775 (*synth, pmr, ir*)
Potapov, V.A. *et al, Zh. Org. Khim.*, 1989, **25**, 1112; *J. Org. Chem. USSR* (*Engl. Transl.*), 1989, **25**, 1001 (*synth*)
Toru, T. *et al, Bull. Chem. Soc. Jpn.*, 1993, **66**, 2042 (*synth, ir, pmr*)

4′-Phenyl-4,2′:6′,4″-terpyridine P-1-00100



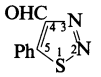
$C_{21}H_{15}N_3$ M 309.3
Complexing reagent. Cryst. Mp 283-284°.

Anderson, H.L. *et al, J.C.S. Perkin 1*, 1995, 2231 (*synth, pmr*)

5-Phenyl-1,2,3-thiadiazole-4-carboxaldehyde, 9CI P-1-00101

4-Formyl-5-phenyl-1,2,3-thiadiazole

[151918-49-9]



$C_9H_6N_2OS$ M 190.2
Cryst. (Et_2O). Mp 54°.

L'abbé, G. *et al, J.C.S. Perkin 1*, 1993, 1719 (*synth, ir, pmr, cmr, ms*)

5-Phenyl-1,5-thiaphosphocane P-1-00102

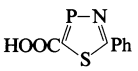
[134021-39-9]

$C_{12}H_{17}PS$ M 224.3
Bidentate ligand for Pd(*II*), Pt(*II*) and Ni(*II*). Oil.

5-Oxide: [134021-38-8].
$C_{12}H_{17}OPS$ M 240.3 Solid.

Toto, S.D. *et al, Inorg. Chem.*, 1990, **29**, 691 (*complexes*)
Toto, S.D. *et al, Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **56**, 27 (*synth, ms, pmr, P-31 nmr, cryst struct*)
Musker, W.K., *Coord. Chem. Rev.*, 1992, **117**, 133 (*rev*)

2-Phenyl-1,3,4-thiazaphosphole-5-carboxylic acid, 9CI P-1-00103



$C_9H_6NO_2PS$ M 223.1

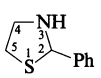
Et ester: [94570-28-2].
$C_{11}H_{10}NO_2PS$ M 251.2 Pale yellow solid. Mp 43-45°.

Schmidpeter, A. *et al, Angew. Chem., Int. Ed.*, 1985, **24**, 123 (*synth, cmr, P-31 nmr*)

2-Phenylthiazolidine P-1-00104

Tetrahydro-2-phenylthiazole

[4569-82-8]



$C_9H_{11}NS$ M 165.2

(±)-*form*
Mp 108-109°.

Térol, A. *et al, Org. Magn. Reson.*, 1981, **17**, 68 (*synth, pmr*)
Baert, F. *et al, Acta Cryst. B*, 1987, **43**, 538 (*cryst struct*)
Umarani, R. *et al, Cryst. Res. Technol.*, 1990, **25**, 1155 (*synth, ir, pmr, cryst struct*)
Barbry, D. *et al, J.C.S. Perkin 2*, 1990, **1**, 133 (*pmr*)
Khumtaveeporn, K. *et al, J.A.C.S.*, 1994, **116**, 5662 (*synth*)

4-Phenylthiazolidine P-1-00105

Tetrahydro-4-phenylthiazole

[107326-18-1]

$C_9H_{11}NS$ M 165.2

(±)-*form*
$Bp_{0.5}$ 120°. Not clear if separated from 5-Phenylthiazolidine, P-1-00106.

Barbry, D. *et al, Chem. Ber.*, 1987, **120**, 1073 (*synth, pmr*)

5-Phenylthiazolidine P-1-00106

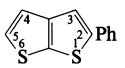
[107326-19-2]

$C_9H_{11}NS$ M 165.2

Barbry, D. *et al, Chem. Ber.*, 1987, **120**, 1073 (*synth, pmr*)
Khumtaveeporn, K. *et al, J.A.C.S.*, 1994, **116**, 5662 (*synth*)

2-Phenylthieno[2,3-*b*]thiophene P-1-00107

[35022-10-7]



$C_{12}H_8S_2$ M 216.3
Mp 166-167°.

Spagnolo, P. *et al, J.C.S. Perkin 1*, 1972, 93.

3-Phenylthieno[2,3-*b*]thiophene P-1-00108

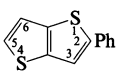
[35022-13-0]

$C_{12}H_8S_2$ M 216.3
Mp 55-56°.

Spagnolo, P. *et al, J.C.S. Perkin 1*, 1972, 93.

2-Phenylthieno[3,2-*b*]thiophene P-1-00109

[35022-09-4]



$C_{12}H_8S_2$ M 216.3
Cryst. (EtOH). Mp 168° (164-166°).

Spagnolo, P. *et al, J.C.S. Perkin 1*, 1972, 93 (*synth*)
Prim, D. *et al, J.C.S. Perkin 1*, 1994, 2603 (*synth, pmr*)

3-Phenylthieno[3,2-*b*]thiophene P-1-00110

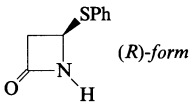
[35022-15-2]

$C_{12}H_8S_2$ M 216.3
Mp 62-63°.

Spagnolo, P. *et al, J.C.S. Perkin 1*, 1972, 93.

4-(Phenylthio)-2-azetidinone, 9CI P-1-00111

[31898-69-8]



(*R*)-*form*

C_9H_9NOS M 179.2
Intermed. for β-lactam antibiotics.

(*R*)-*form* [85270-00-4]
Cryst. (CH_2Cl_2/petrol). Mp 68-69°. $[\alpha]_D$ +137.3 (c, 1.29 in $CHCl_3$).

(*S*)-*form* [90497-62-4]
Cryst. (Et_2O/hexane). $[\alpha]_D^{25}$ −134.6 (c, 1.21 in $CHCl_3$).

(±)-*form* [106974-96-3]
Cryst. (MeOH). Mp 72-73.5°.

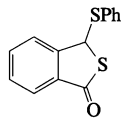
S-*Oxide:* [53390-58-2]. *4-(Phenylsulfinyl)-2-azetidinone, 9CI*
$C_9H_9NO_2S$ M 195.2 Cryst. (hexane/CH_2Cl_2). Mp 107-108°, Mp 124-127°.

S,S-*Dioxide:* [90497-61-3]. *4-(Phenylsulfonyl)-4-azetidinone*
$C_9H_9NO_3S$ M 211.2 Cryst. (H_2O). Mp 156-157°.

[31899-01-1, 99746-85-7]

Clauss, K. *et al, Annalen*, 1974, 539 (*synth, ir, pmr*)
Nishida, A. *et al, Tet. Lett.*, 1984, **25**, 765 (*synth*)
Gu, H. *et al, J.O.C.*, 1990, **55**, 5655 (*synth*)
Kita, Y. *et al, Chem. Pharm. Bull.*, 1992, **40**, 1044 (*synth, ir, pmr, sulfoxide*)
Iwata-Renyl, D. *et al, J. Nat. Prod.*, 1993, **56**, 1373 (*synth, pmr, cmr, ms*)
Basak, A. *et al, Synth. Commun.*, 1994, **24**, 131 (*synth*)

3-(Phenylthio)benzo[*c*]thiophen-1(3*H*)-one P-1-00112



$C_{14}H_{10}OS_2$ M 258.3

(±)-*form* [155988-85-5]
Cryst. Mp 57°.

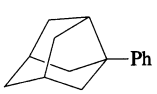
S′,S′-*Dioxide:* [155988-86-6]. *3-(Phenylsulfonyl)benzo*[c]*thiophen-1*(3H)*-one*
$C_{14}H_{10}O_3S_2$ M 290.3 Cryst. (Et_2O/petrol). Mp 165-167°.

Majumdar, G. *et al, J.C.S. Perkin 1*, 1994, 309.

3-Phenyltricyclo[3.3.1.0^{3,7}]nonane P-1-00113

Octahydro-3a-phenyl-2,5-methanopentalene, 9CI. 3-Phenylnoradamantane

[151697-56-2]



$C_{15}H_{18}$ M 198.3
Liq. Bp_2 92°.

Olah, G.A. *et al, J.A.C.S.*, 1993, **115**, 10728 (*synth, pmr, cmr, ms*)

Phenylvinylphosphinous acid, 8CI P-1-00114

Ethenylphenylphosphinous acid, 9CI

$H_2C{=}CHPPhOH$

C_8H_9OP M 152.1

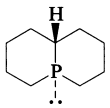
Butyl ester: [77085-88-2]. *Butyl ethenylphenylphosphinite*
$C_{12}H_{17}OP$ M 208.2 Liq. d_4^{20} 0.98. Bp_2 76-77°. n_D^{20} 1.5310.

Kabachnik, M.I. *et al, Zh. Obshch. Khim.*, 1962, **32**, 3351.
Kharrasova, F.M. *et al, Zh. Obshch. Khim.*, 1968, **38**, 359.

1-Phosphabicyclo[4.4.0]decane P-1-00115

Octahydro-2H-phosphinolizine

[88580-67-0]



(1*RS*,6*RS*)-*form*

$C_9H_{17}P$ M 156.2

(*1RS,6RS*)-*form* [118333-78-1]
trans-*form*
Liq. Bp_{10} 87°.

Methiodide:
$C_{10}H_{20}IP$ M 298.1 Solid. Mp 305-306°.

P-*Oxide:* [118375-04-5].
$C_9H_{17}OP$ M 172.2 Solid. Mp 154-156°.

P-*Sulfide:* [118375-05-6].
$C_9H_{17}PS$ M 188.2 Solid. Mp 132-133°.

P-*Selenide:* [118375-06-7].
$C_9H_{17}PSe$ M 235.1 Solid. Mp 154-155°.

(*1RS,6SR*)-*form* [118333-79-2]
cis-*form*
Liq. $Bp_{1.2}$ 63°. Forms a CS_2 adduct.

Methiodide: Octahydro-5-methylphosphinolizinium iodide
Solid. Mp 384-386°.

P-*Oxide:* [118266-97-0].
Solid. Mp 103-104.5°.

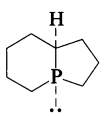
P-*Sulfide:* [118281-63-3].
Solid. Mp 66-67°.

P-*Selenide:* [118281-64-4].
Solid. Mp 93-95°.

Krech, F. *et al, Z. Anorg. Allg. Chem.*, 1987, **553**, 136 (*synth, cmr, P-31 nmr, Se-77 nmr*)

1-Phosphabicyclo[4.3.0]nonane P-1-00116

Octahydrophosphindolizine, 9CI



$C_8H_{15}P$ M 142.1

(*1RS,6SR*)-*form* [137564-97-7]
(±)-cis-*form*
Liq. Bp_{11} 83-84°.

Methiodide: [137565-00-5]. *1-Methyloctahydrohydrophosphindolizinium iodide*
$C_9H_{18}IP$ M 284.1 Cryst. (EtOH). Mp 388-391° dec.

Hydrogen fluorosulfate: [137564-99-9].
$C_8H_{16}FO_4PS$ M 258.2 Props. not reported.

Oxide: [137593-49-8].
$C_8H_{15}OP$ M 158.1 Oil. $Bp_{0.02}$ 103-105°.

Sulfide: [137565-01-6].
$C_8H_{15}PS$ M 174.2 Cryst. (Et_2O). Mp 56-58°.

Selenide: [137565-02-7].
$C_8H_{15}PSe$ M 221.1 Cryst. (Et_2O/pentane). Mp 59-61°.

CS_2 adduct: Solid. Dec. at 69-73°.

Krech, F. *et al, Z. Anorg. Allg. Chem.*, 1991, **600**, 195 (*synth, cmr, P-31 nmr, Se-77 nmr*)

Phosphetanic acid P-1-00117

1-Hydroxyphosphetane 1-oxide

[117961-78-1]

$C_3H_7O_2P$ M 106.0
Waxy solid.

Me ester: [150786-93-9]. *1-Methoxyphosphetane 1-oxide. Methyl phosphetanate*
$C_4H_9O_2P$ M 120.0 Oil.

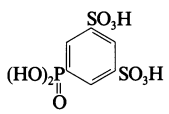
Et ester: 1-Ethoxyphosphetane 1-oxide. Ethyl phosphetanate
$C_5H_{11}O_2P$ M 134.1 Liq. Bp_{10} 95-102°.

Kosolapoff, G.M. *et al, J.C.S.*, 1957, 3739.
Wong, S.-C. *et al, J. Chem. Res., Synop.*, 1993, 268 (*synth, ester, ms, ir, pmr, cmr, P-31 nmr*)

5-Phosphono-1,3-benzenedisulfonic acid P-1-00118

Phenylphosphonic acid 3,5-disulfonic acid

[126766-74-3]

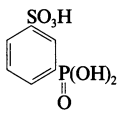


$C_6H_7O_9PS_2$ M 318.2
Obt. from Phenylphosphonic acid, P-0-02344 by sulfonation (SO_3 at 180-240°). Solid. Mp 146°.

Montoneri, E., *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **55**, 201; 1994, **86**, 123 (*synth, pmr, cmr, P-31 nmr*)

3-Phosphonobenzenesulfonic acid P-1-00119

[126180-64-1]



$C_6H_7O_6PS$ M 238.1
Obt. from Phenylphosphonic acid, P-0-02344 by sulfonation with SO_3. Solid. Mp 164°.

Montoneri, E. *et al, J.C.S. Dalton*, 1989, 1819 (*synth, ir, pmr, cmr, P-31 nmr*)
Montoneri, E., *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **55**, 201; 1994, **86**, 123 (*synth, pmr, cmr, P-31 nmr*)

2-Phosphonoethanesulfonic acid P-1-00120

[75407-14-6]

$HO_3SCH_2CH_2P(O)(OH)_2$

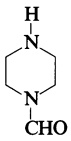
$C_2H_7O_6PS$ M 190.1
Hydrated solid. Mp 156°. Stable to 200°.

Doi, J.T. *et al, Phosphorus Sulfur Relat. Elem.*, 1988, **35**, 173 (*salt, synth, ir, pmr, P-31 nmr*)
Montoneti, E. *et al, Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **55**, 111 (*synth, ir, pmr, P-31 nmr*)

1-Piperazinecarboxaldehyde, 9CI P-1-00121

N-*Formylpiperazine*

[7755-92-2]



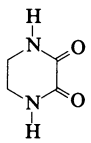
$C_5H_{10}N_2O$ M 114.1
Liq. d 1.11. $Bp_{0.5}$ 94.7°.

Horrom, B.W. *et al, J.A.C.S.*, 1955, **77**, 753 (*synth*)

2,3-Piperazinedione, 9CI P-1-00122

2,3-Diketopiperazine

[13092-86-9]



$C_4H_6N_2O_2$ M 114.1
Solid. Mp 285° dec.

1-Et: [59702-31-7].
$C_6H_{10}N_2O_2$ M 142.1 Coml. available synth. intermediate.

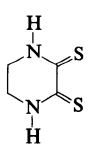
1,4-Di-Me: [59417-06-0].
$C_6H_{10}N_2O_2$ M 142.1 Reacts with organometallic reagents to give α-diketones. Cryst. (PhMe). Mp 178-179°.

1,4-Didecyl: [156909-31-8].
$C_{24}H_{46}N_2O_2$ M 394.6 Reagent for the synth. of unsym. α-diketones. Cryst. (hexane). Mp 114-116°.

[59702-29-3]

Goulding, C.E. *et al, J.A.C.S.*, 1948, **70**, 1967 (*synth*)
Saikawa, I. *et al, Yakugaku Zasshi*, 1977, **97**, 980; *CA*, **88**, 105210p (*synth, monoalkyl derivs*)
Japan. Pat., 81 77 226, (1981); *CA*, **95**, 203994m (*synth, monoalkyl derivs*)
Mueller-Westerhoff, U.T. *et al, J.O.C.*, 1994, **59**, 4988 (*synth, pmr, cmr, ms, use, dialkyl derivs*)

2,3-Piperazinedithione P-1-00123



$C_4H_6N_2S_2$ M 146.2

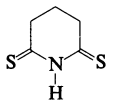
N,N′-*Di-Me:*
$C_6H_{10}N_2S_2$ M 174.2 Dark red needles (EtOH). Mp 228-230°.

Isaksson, R. *et al, J. Chem. Res., Miniprint*, 1981, 664; *J. Chem. Res., Synop.*, 1981, 43.

2,6-Piperidinedithione, 9CI P-1-00124

Dithioglutarimide, 8CI

[5695-94-3]

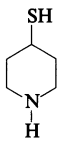


$C_5H_7NS_2$ M 145.2
Orange-yellow cryst. (MeOH aq.). Mp 112°.

Berg, U. *et al, Acta Chem. Scand.*, 1966, **20**, 689 (*synth, uv*)
Hoffmann, R. *et al, Annalen*, 1977, 1743 (*synth, ir, pmr*)
Gossauer, A. *et al, Annalen*, 1979, 1309 (*synth*)

4-Piperidinethiol, 9CI P-1-00125

4-Mercaptopiperidine

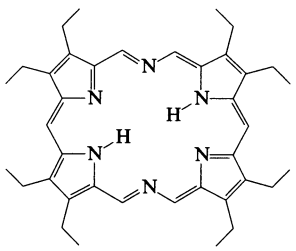


$C_5H_{11}NS$ M 117.2
Hydrochloride: [99201-86-2].
Cryst. (EtOH).
1-Me: [1072-99-7].
$C_6H_{13}NS$ M 131.2 Oil. $Bp_{0.8}$ 62°, $Bp_{0.04\text{-}0.05}$ 30-35°.
1-Me, hydrochloride: Cryst. Mp 172-173°.

Barrera, H. *et al, J.O.C.*, 1962, **27**, 641 (*1-Me, synth*)
Engel, J. *et al, Arch. Pharm. (Weinheim, Ger.)*, 1988, **321**, 821 (*synth, pmr*)
Meanwell, N.A. *et al, J. Med. Chem.*, 1993, **36**, 3251 (*1-Me, synth, ir, pmr*)

Porphocyanine P-1-00126

[150990-73-1]



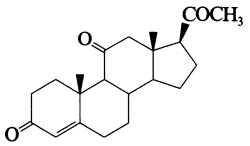
$C_{38}H_{48}N_6$ M 588.8
Green solid.

Dolphin, D. *et al, J.A.C.S.*, 1993, **115**, 9301 (*synth, pmr, uv-vis*)
Xie, L.Y. *et al, Chem. Comm.*, 1994, 1475 (*synth*)

Pregn-4-ene-3,11,20-trione, 9CI P-1-00127

Updated Entry replacing P-0-03138
11-Oxoprogesterone. Ketogestin. Bio. 66. U 1258

[516-15-4]



$C_{21}H_{28}O_3$ M 328.4
Formerly used in the treatment of bovine acetonaemia. Anaesthetic. Cryst. (Me_2CO/petrol). Mp 174.5-175.5° (171.5-173°). $[\alpha]_D^{25}$ +270 ($CHCl_3$).

▶ Exp. reprod. effects. TU5513000.

[81800-93-3]

Reichstein, T. *et al, Helv. Chim. Acta*, 1940, **23**, 688 (*synth*)
Ger. Pat., 1 111 179, (1959) (*Upjohn*); *CA*, **56**, 4829 (*synth*)
Huang, S.L. *et al, Synthesis*, 1978, 297 (*synth*)
Razzak, K.S.A. *et al, Biomed. Mass Spectrom.*, 1980, **7**, 505 (*ms*)
Stork, G. *et al, J.A.C.S.*, 1982, **104**, 3758 (*synth*)
Ziegler, F.E. *et al, J.A.C.S.*, 1984, **106**, 718 (*synth*)
Nemoto, H. *et al, J.C.S. Perkin 1*, 1986, 1621 (*synth*)
Gupta, V.K. *et al, Acta Cryst. C*, 1994, **50**, 798 (*cryst struct*)

1,3-Propanediphosphonous acid P-1-00128

1,3-Propanediylbisphosphonous acid, 9CI. Trimethylenebisphosphonous acid, 8CI

$(HO)_2PCH_2CH_2CH_2P(OH)_2$

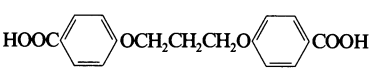
$C_3H_{10}O_4P_2$ M 172.0
Bis(dichloride): [28240-70-2].
$C_3H_6Cl_4P_2$ M 245.8 Pungent liq. Bp_2 93°. Easily hydrol.
Bis(dibromide): [86926-35-4].
$C_3H_6Br_4P_2$ M 423.6 Pungent liq. $Bp_{0.1}$ 112°. Easily hydrol.

Sommer, K., *Z. Anorg. Allg. Chem.*, 1970, **376**, 37 (*chloride, synth, P-31 nmr*)
Diemert, K. *et al, Chem. Ber.*, 1982, **115**, 1947 (*bromide, synth, P-31 nmr*)

4,4′-[1,3-Propanediylbis(oxy)] bisbenzoic acid P-1-00129

4,4′-(Trimethylenedioxy)dibenzoic acid. 1,3-Diphenoxypropane-p,p′-dicarboxylic acid

[3753-81-9]



$C_{17}H_{16}O_6$ M 316.3
Insol. H_2O. Mp 332-334° (310-312°).

Polymer with decanedioic acid: [90409-78-2].
Polifeprosan, INN. *Polifeprosan 20, USAN. PCPP-SA. Biodel*
Biodegradable polyanhydride used as a drug-carrier matrix for controlled delivery applications.

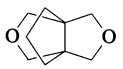
McMillan, F.H., *J.A.C.S.*, 1952, **74**, 5229 (*synth*)

Donahoe, H.B. *et al*, *J.O.C.*, 1961, **26**, 474 (*synth*)
Leong, K.W. *et al*, *Polym. Prepr.*, (*Am. Chem. Soc., Div. Polym. Chem.*), 1984, **25**, 201 (*synth, polifeprosan*)
Leong, K.W. *et al*, *J. Biomed. Mater. Res.*, 1985, **19**, 941 (*use, polifeprosan*)
Domb, A.J. *et al*, *Polym. Mater. Sci. Eng.*, 1986, **55**, 746 (*synth, polifeprosan*)
Ron, E. *et al*, *Macromolecules*, 1991, **24**, 2278 (*pmr, cryst struct, polifeprosan*)
Tudor, A.M. *et al*, *Spectrochim. Acta A*, 1991, **47**, 1335 (*polifeprosan, ir, Raman*)
Domb, A.J., *Macromolecules*, 1992, **25**, 12 (*synth, polifeprosan*)

4*H*,6*H*-3*a*,6*a*-Propano-1*H*,3*H*-furo[3,4-*c*]furan, 9CI, 8CI P-1-00130

3,7-Dioxa[3.3.3]propellane

[17853-49-5]



$C_9H_{14}O_2$ M 154.2
Mp 155-157° (129-132°).

Altman, J. *et al*, *Tetrahedron*, 1967, **24**, 975 (*synth, ir, pmr*)
Weinges, K. *et al*, *Annalen*, 1971, **746**, 70 (*synth*)

Propanoic acid, 9CI P-1-00131

Updated Entry replacing P-0-03261

Propionic acid. Metacetonic acid. Ethanecarboxylic acid

[79-09-4]

H_3CCH_2COOH

$C_3H_6O_2$ M 74.0

Volatile component of human vaginal secretions. Gut flora metabolite, found in faeces. Manuf. by oxidation of naphtha or butane. Food preservative used esp. in bread and grain mold inhibitors. Also used in cellulose propionate manuf. Antifungal agent (and salts). Liq. with acrid odour. Misc. H_2O. d_{15}^{15} 0.999. Mp −21.5°. Bp 141.1°, Bp_{10} 39.7°. Simple esters used as flavouring agents.

▶ Corrosive and mod. irritating to skin, eyes and respiratory tract. LD_{50} (rat, orl) 3500 mg/kg. OES: long-term 10 ppm; short-term 15 ppm. UE5950000.

NH_4 salt: [17496-08-1].
V. hygroscopic cryst. Mp 45°.

K salt: [327-62-8].
Plates + $1H_2O$ (EtOH aq.). Mp >300°.

Me ester: [554-12-1]. *Methyl propionate*
$C_4H_8O_2$ M 88.1 Liq. d_4^0 0.939. Bp 79.7°. n_D^{19} 1.3770.
▶ Highly flammable, fl. p. −2°, autoignition temp. 469°. Skin irritant. UF5970000.

Et ester: [105-37-3]. *Ethyl propionate*
$C_5H_{10}O_2$ M 102.1 Water scavenger for alkoxide-catalysed condensations. Used in fruity and rum flavour compositions. Liq. with fruity odour. Mod. sol. H_2O. d_4^{20} 0.891. Fp −73°. Bp 99°. n_D^{20} 1.3844.
▶ Flammable, fl. p. 12°, autoignition temp. 440/476°. Skin irritant. UF3675000.

Vinyl ester: [105-38-4].
$C_5H_8O_2$ M 100.1 Manuf. from acetylene + propanoic acid. Monomer for radical polym. Liq. Insol. H_2O. d^{20} 0.9203. n_D^{20} 1.4003. Q/e values for copolym., Q 0.027, e −0.68.

Propyl ester: [106-36-5]. *Propyl propionate*
$C_6H_{12}O_2$ M 116.1 Liq. d^0 0.893. Bp 122°.
▶ Fl. p. 79° (oc). Skin irritant. UF7100000.

Isopropyl ester: [637-78-5]. *Isopropyl propionate*
$C_6H_{12}O_2$ M 116.1 Liq. d^0 0.893. Bp_{750} 109-111°.
▶ Highly flammable, fl. p. 21°. UF5140000.

Butyl ester: [590-01-2]. *Butyl propionate*
$C_7H_{14}O_2$ M 130.1 Liq. d_0^0 0.893. Bp 145.5°.
▶ Flammable, fl. p. 32°, autoignition temp. 426°. Skin irritant. UE8245000.

1-Methylpropyl ester: [591-34-4]. *1-Methylpropyl propanoate.* sec-*Butyl propionate*
$C_7H_{14}O_2$ M 130.1 Liq. d_4^{20} 0.866. Bp 132°. n_D^{25} 1.3938.

2-Methylpropyl ester: [540-42-1]. *2-Methylpropyl propanoate. Isobutyl propionate*
$C_7H_{14}O_2$ M 130.1 Liq. d_4^0 0.888. Bp 137°.
▶ Highly flammable, fl. p. 18°. UF4930000.

tert-*Butyl ester:* [20487-40-5]. tert-*Butyl propionate*
$C_7H_{14}O_2$ M 130.1 Liq. Bp 117-119°.

Pentyl ester: [624-54-4]. *Pentyl propanoate. Amyl propionate*
$C_8H_{16}O_2$ M 144.2 Liq. d_4^{15} 0.876. Fp −73.1°. Bp 168.7°. n_D^{15} 1.4096.

Benzyl ester: [122-63-4]. *Benzyl propionate*
$C_{10}H_{12}O_2$ M 164.2 Liq. Bp 222°.

Ph ester: [637-27-4]. *Phenyl propionate*
$C_9H_{10}O_2$ M 150.1 Prisms. Mp 20°. Bp 211°.
▶ Fl. p. 86°.

Fluoride: [430-71-7]. *Propionyl fluoride*
C_3H_5FO M 76.0 Liq. Bp 44°.

Chloride: [79-03-8]. *Propionyl chloride*
C_3H_5ClO M 92.5 Liq. Bp 80°.
▶ Highly flammable, fl. p. 12°. Corrosive and irritating to skin, eyes and mucous membranes. Reacts violently with H_2O. UG6657000.

Bromide: [598-22-1]. *Propionyl bromide*
C_3H_5BrO M 136.9 Liq. d^{16} 1.521. Bp 103-103.6°. n_D^{16} 1.4578.

Iodide: [598-40-3]. *Propionyl iodide*
C_3H_5IO M 183.9 Yellowish liq. Bp 127-128°, Bp_{30} 75°, Bp_{50} 52-53°.

Amide: [79-05-0]. *Propanamide, 9CI. Propionamide*
C_3H_7NO M 73.0 Plates (C_6H_6). Mp 79°. Bp 222.2°. Steam-volatile.

Amide, N-*Ac:* [19264-34-7].
$C_5H_9NO_2$ M 115.1 Mp 86°. Bp 230-240°.

Methylamide: [1187-58-2].
d 0.93. Mp −43°. Bp_{90} 146°. n_D^{20} 1.4360.

Dimethylamide: [758-96-3].
$C_5H_{11}NO$ M 101.1 Liq. Bp 165-178°.
▶ UE3810000.

Diethylamide: [1114-51-8].
$C_7H_{15}NO$ M 129.2 Bp_{12} 77°. n_D^{20} 1.4420.

Anilide: [620-71-3]. *Propionanilide*
$C_9H_{11}NO$ M 149.1 Cryst. (C_6H_6). Bp 104-104.5°.

Hydrazide: [5818-15-5].
$C_3H_8N_2O$ M 88.1 Sol. H_2O; spar. sol. Et_2O. Mp 40°. Bp_{16} 130°.

Nitrile: [107-12-0]. *Propionitrile. Ethyl cyanide. Cyanoethane*
C_3H_5N M 55.0 Liq. with ethereal odour. Part. misc. H_2O. Fp −103.5°. Bp 97°.
▶ Rapidly absorbed through skin. One of the most toxic organic cyanides known. Highly flammable, fl. p. 2°. Skin and eye irritant. LD_{50} (rat, orl) 39 mg/kg. LD_{50} (rbt, skn) 210 mg/kg. LC_{50} (mus, ihl) 163 ppm (1h exposure). UF6250000.

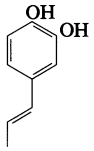
Anhydride: [123-62-6]. *Propionic anhydride*
$C_6H_{10}O_3$ M 130.1 Liq. Bp 168.4-168.8°, Bp_{18} 67.5°.
▶ Flammable. Corrosive and irritating to skin, eyes and mucous membranes. UF9100000.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **1**, 751C, 904A, 904B, 904C, 905A, 905B, 905C, 1165C, 1188B, 1188C, 1219A, 1235A, 1243C, 1244A, 1351B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 27C, 481D, 603D, 604A, 604B, 711B, 724D, 747C, 761A, 837B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 573D, 611C, 611D, 612A, 612B, 612C, 612D, 761A, 766D, 777C, 781A, 783C, 783D, 795B (*ir*)
Hardy, D.V.N. *et al*, *J.C.S.*, 1936, 358, 364 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 2nd edn., Wiley, New York, 1963-1971, **16**, 554 (*rev*)
Crispin, P.D. *et al*, *Aust. J. Chem.*, 1967, **20**, 2589 (*amide*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 385 (*ester*)
Bevington, J.C. *et al*, *Eur. Polym. J.*, 1968, **4**, 373 (*polym, vinyl ester*)
Ger. Pat., 2 324 765, (1974); *CA*, **80**, 70359z (*ester*)
Michael, R.P. *et al*, *Science* (*Washington, D.C.*), 1974, **186**, 1217 (*sex attractant*)
Mondal, M.A.S. *et al*, *Tetrahedron*, 1974, **30**, 4205 (*synth, vinyl ester*)
Williamson, K.L. *et al*, *J. Magn. Reson.*, 1978, **30**, 367 (*cmr*)
Greenley, R.Z., *J. Macromol. Sci., Chem., Part A*, 1980, **14**, 427 (*Q/e values, vinyl ester*)
Maccoll, A., *Int. J. Mass Spectrom. Ion Processes*, 1988, **86**, 227 (*ms*)
Lewis, R.J., *Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, EPB500, PMU750.
Keinan, E. *et al*, *J.O.C.*, 1990, **55**, 3922 (*iodide*)
Edwards, H.G.M. *et al*, *J. Mol. Struct.*, 1991, **248**, 237 (*ir, Raman*)
Yokoyama, I. *et al*, *Bull. Chem. Soc. Jpn.*, 1993, **66**, 400 (*ir, Raman*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 331.
Yang, H. *et al*, *Synth. Commun.*, 1994, **24**, 3269 (*esters*)
Patty's Ind. Hyg. Toxicol. (*3rd Rev. edn.*), Vol. 2, Wiley, 1980, 4911.
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BSJ500, EPB500, MOT000, PMU750, PMV000, PMV250, PMV500, PMV750, PMW500, PNU000.
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (Snyder, R., Ed.), Elsevier, Volume 2, 1990, 354 (*propionitrile*)

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworth, London and Boston, 1990, 1092, 1108, 1520, 1849, 2350, 2677.
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 1068, 1069.

4-(1-Propenyl)-1,2-benzenediol, 9CI P-1-00132

[72898-29-4]



$C_9H_{10}O_2$ M 150.1
Isol. (as di-Me ether) from *Solidago* sp.

(E)-form

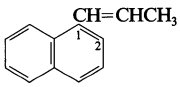
2-Et ether: [63477-41-8]. *2-Ethoxy-5-(1-propenyl)phenol, 9CI. Isosafroeugenole. Propenylguaethole*
$C_{11}H_{14}O_2$ M 178.2 Mp 86-88°.

[94-86-0]

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1027D (*ir*)
Aldrich Library of NMR Spectra, **1**, 886C (*pmr*)
Bohlmann, F. *et al, Phytochemistry*, 1980, **19**, 2655 (*isol*)
Klungsoeyr, J. *et al, Biomed. Mass Spectrom.*, 1982, **9**, 323 (*metab, glc*)
Radhakrishna, A.S. *et al, Synth. Commun.*, 1991, **21**, 379 (*synth*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th Ed., Van Nostrand-Reinhold, 1992, IRY000.

1-(1-Propenyl)naphthalene, 9CI P-1-00133

[22767-77-7]



$C_{13}H_{12}$ M 168.2
Yellow oil. Bp_{10} 139-140°. Pure *E*- and *Z*-isomers have not been reported.

[53269-00-4, 53269-01-5]

Fieser, L.F. *et al, J.A.C.S.*, 1938, **60**, 1658 (*synth*)
Kon, G.A.R. *et al, J.C.S.*, 1949, 2725 (*synth*)
Bohlmann, F. *et al, Tetrahedron*, 1974, **30**, 1011 (*ms*)
Boudjouk, P. *et al, J. Organomet. Chem.*, 1978, **155**, C13 (*synth, pmr*)
Anderson, J.E. *et al, J.C.S. Perkin 2*, 1987, 955 (*pmr, conformn*)

2-(1-Propenyl)naphthalene, 9CI P-1-00134

[51051-94-6]

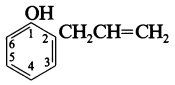
$C_{13}H_{12}$ M 168.2
Solid. Mp 28°. Config. not given.

Kon, G.A.R. *et al, J.C.S.*, 1949, 2725 (*synth*)

2-(2-Propenyl)phenol, 9CI P-1-00135

2-Allylphenol

[1745-81-9]



$C_9H_{10}O$ M 134.1
Liq. Bp_{16} 106°, $Bp_{3.5}$ 78-80°.

Bruce, J.M. *et al, J.C.S. Perkin 1*, 1981, 2677 (*synth*)
Bigi, F. *et al, Synthesis*, 1981, 310 (*synth*)
Alberola, A. *et al, J.C.S. Perkin 1*, 1983, 1209 (*synth, pmr*)

3-(2-Propenyl)phenol, 9CI P-1-00136

3-Allylphenol

[1446-24-8]

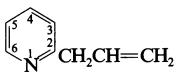
$C_9H_{10}O$ M 134.1
Liq.

Kitamura, T. *et al, Tetrahedron*, 1978, **34**, 3451 (*synth, pmr*)

2-(2-Propenyl)pyridine, 9CI P-1-00137

2-Allylpyridine

[2835-33-8]



C_8H_9N M 119.1
Liq. Bp_{12} 63-65°.

Picrate: Yellow cryst. (EtOH). Mp 121.5-122°, Mp 157-161°.

Gilman, H. *et al, J.A.C.S.*, 1957, **79**, 1245 (*synth*)
Wibaut, J.P. *et al, Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1958, **77**, 123 (*synth*)
Yingst, R.E. *et al, Inorg. Chem.*, 1964, **3**, 1177 (*synth*)
Hanessian, S. *et al, Synthesis*, 1987, 409 (*synth, ir, pmr*)

3-(2-Propenyl)pyridine, 9CI P-1-00138

3-Allylpyridine

[7300-28-9]

C_8H_9N M 119.1
Liq. Bp_{18} 78°.

Picrate: Cryst. Mp 109.2-109.6°.

Wibaut, J.P. *et al, Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1952, **71**, 798 (*synth*)
Ishikura, M. *et al, Heterocycles*, 1985, **23**, 117 (*synth*)
Ishikura, M. *et al, J. Het. Chem.*, 1987, **24**, 377 (*synth, ir, pmr*)

4-(2-Propenyl)pyridine, 9CI P-1-00139

4-Allylpyridine

[80880-49-5]

C_8H_9N M 119.1
Liq. Bp_{18} 90°.

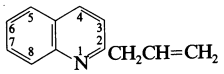
Picrate: Cryst. Mp 167.5-168.5°.

Gilman, H. *et al, J.A.C.S.*, 1957, **79**, 1245 (*synth*)
Ishikura, M. *et al, J. Het. Chem.*, 1987, **24**, 377 (*synth, ir, pmr*)

2-(2-Propenyl)quinoline, 9CI P-1-00140

2-Allylquinoline

[33328-29-9]



$C_{12}H_{11}N$ M 169.2
Oil. Attempts at purifn. lead to mixts. with (*E*)- and (*Z*)-2-(1-propenyl)quinoline.

Thorsett, E.D. *et al, J. Het. Chem.*, 1973, **10**, 243 (*synth, pmr*)
Wakabayashi, S. *et al, Bull. Chem. Soc. Jpn.*, 1989, **62**, 2338 (*synth, pmr*)

3-(2-Propenyl)quinoline, 9CI P-1-00141

3-Allylquinoline

[111678-25-2]

$C_{12}H_{11}N$ M 169.2
Bp_1 110°.

Picrate: [111678-66-1]. Mp 179-180°.

Ishikura, M. *et al, J. Het. Chem.*, 1987, **24**, 377 (*synth, ir, pmr*)

4-(2-Propenyl)quinoline, 9CI P-1-00142

4-Allylquinoline

[59647-04-0]

$C_{12}H_{11}N$ M 169.2

Akiba, K. *et al, Tet. Lett.*, 1982, **23**, 1709 (*synth*)

8-(2-Propenyl)quinoline, 9CI P-1-00143

8-Allylquinoline

[73038-02-5]

$C_{12}H_{11}N$ M 169.2
Oil.

Suggs, J.W. *et al, J.O.C.*, 1980, **45**, 1514 (*synth, ir, pmr*)

4-Propyl-4-heptylamine P-1-00144

4-Propyl-4-heptanamine, 9CI. 1,1-Dipropylbutylamine. Tripropylmethylamine. Diprobutine, INN, BAN

[61822-36-4]

$(H_3CCH_2CH_2)_3CNH_2$

$C_{10}H_{23}N$ M 157.2
Exhibits anticholinergic activity. Antiparkinsonian agent. Never marketed.
▶ LD_{50} (rat, orl) 135 mg/kg. LD_{50} (rat, ipr) 23 mg/kg. MI7630000.

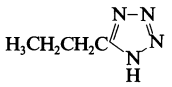
Hydrochloride: [56065-37-3]. *LCG 21519* Cryst. Mp 220° subl.
▶ MI7632000.

Fumarate: Mp 216° subl.

Belg. Pat., 834 298, (1976) (*Labaz*); *CA*, **86**, 71886e (*synth, pharmacol*)
Pigerol, C. *et al, Eur. J. Med. Chem. (Chim. Ther.)*, 1977, **12**, 351 (*synth, pharmacol*)
Hillier, K. *et al, Drugs of the Future*, 1978, **3**, 454 (*rev*)
Chemouilli, P. *et al, Eur. J. Pharmacol.*, 1985, **117**, 205 (*pharmacol*)
Davies, C.L. *et al, J. Chromatogr.*, 1985, **339**, 186 (*glc*)

5-Propyl-1*H*-tetrazole, 9CI P-1-00145

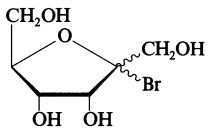
[14389-13-0]



$C_4H_8N_4$ M 112.1
Waxy solid. Mp 63-64° (56-58°).

Finnegan, W.G. *et al, J.A.C.S.*, 1958, **50**, 3908 (*synth*)
Thomas, E.W. *et al, Synthesis*, 1993, 767 (*synth, pmr, ir, ms*)

Psicofuranosyl bromide P-1-00146



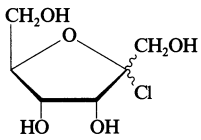
$C_6H_{11}BrO_5$ M 243.0

D-form

Tetrabenzoyl: [54401-10-4].
$C_{34}H_{27}BrO_9$ M 659.4 Semi-cryst.

Prisbe, E.J. *et al, J.O.C.*, 1976, **41**, 1836 (*tetrabenzoyl*)

Psicofuranosyl chloride P-1-00147



D-Furanose-*form*

$C_6H_{11}ClO_5$ M 198.6

D-form

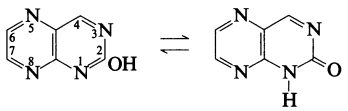
Tetrabenzoyl: [13019-85-7].
$C_{34}H_{27}ClO_9$ M 615.0 Syrup.

Grouiller, A. *et al, Acta Chem. Scand., Ser. B*, 1984, **38**, 367 (*tetrabenzoyl*)

2-Pteridinol P-1-00148

2(1H)-Pteridinone, 9CI. 2-Hydroxypteridine

[2432-24-8]



$C_6H_4N_4O$ M 148.1
Adds water reversibly; exists predominantly as a covalent hydrate of 1*H*-oxo-form.

Monohydrate: 3,4-Dihydro-4-hydroxy-2(1H)-pteridinone. 3,4-Dihydro-2,4-dihydroxypteridine
$C_6H_6N_4O_2$ M 166.1 Needles (H_2O). Mp 240° dec.

[25911-76-6]

Albert, A. *et al, J.C.S.*, 1951, 474 (*synth*)
Brown, D.J. *et al, J.C.S.*, 1956, 3443 (*ir, uv, tautom*)
Inoue, Y. *et al, J.C.S.*, 1962, 2600 (*uv*)

6-Pteridinol P-1-00149

6(5H)-Pteridinone, 9CI. 6-Hydroxypteridine

[2432-26-0]

$C_6H_4N_4O$ M 148.1
Adds water reversibly; exists predominantly as a covalent hydrate of 5*H*-6-oxo-form.

Monohydrate: [10577-47-6]. *7,8-Dihydro-7-hydroxy-6(5H)-pteridinone, 9CI. 7,8-Dihydro-6,7-dihydroxypteridine*
$C_6H_6N_4O_2$ M 166.1 Cryst. (H_2O).

Albert, A. *et al, J.C.S.*, 1952, 1620; 1955, 2690 (*synth*)
Brown, D.J. *et al, J.C.S.*, 1956, 3443 (*ir, uv, tautom*)
Inoue, Y. *et al, J.C.S.*, 1962, 2600 (*uv, hydration*)

7-Pteridinol P-1-00150

7(8H)-Pteridinone, 9CI. 7-Hydroxypteridine

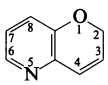
[2432-27-1]

$C_6H_4N_4O$ M 148.1
Cryst. (H_2O). Dec. slowly >230°.

Albert, A. *et al, J.C.S.*, 1952, 1620; 1956, 4621 (*synth*)
Brown, D.J. *et al, J.C.S.*, 1956, 3443 (*ir, uv, tautom*)

2*H*-Pyrano[3,2-*b*]pyridine, 9CI P-1-00151

[4767-91-3]

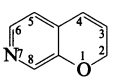


C_8H_7NO M 133.1
Oil. Bp_1 63°.

Bruhn, J. *et al, Helv. Chim. Acta*, 1978, **61**, 2542 (*synth, pmr, uv, ms*)
Sliwa, H. *et al, Heterocycles*, 1979, **12**, 493 (*synth, pmr, ir*)
Sliwa, H. *et al, Synthesis*, 1993, 881 (*synth, pmr, cmr, ir, ms*)

2*H*-Pyrano[2,3-*c*]pyridine, 9CI P-1-00152

[767-93-1]

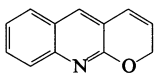


C_8H_7NO M 133.1
Bp_4 95°. n_D^{20} 1.5906.

Sliwa, H. *et al, Tet. Lett.*, 1991, **32**, 627 (*synth*)
Sliwa, H. *et al, Synthesis*, 1993, 881 (*synth, pmr, cmr, ir, ms*)

2*H*-Pyrano[2,3-*b*]quinoline P-1-00153

[261-03-0]



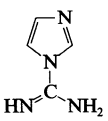
$C_{12}H_9NO$ M 183.2
Mp 144-146°.

Cziáky, Z. *et al, J. Het. Chem.*, 1994, **31**, 701.

1*H*-Pyrazole-1-carboximidamide, 9CI P-1-00154

1-Guanylpyrazole. Pyrazole-1-carboxamidine. ***Praxadine, INN***

[4023-00-1]



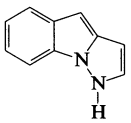
$C_4H_6N_4$ M 110.1
Analgesic, antiinflammatory agent. Never marketed. Mp 97-101°.

Hydrochloride: [4023-02-3].
Cryst. (H_2O). Mp 170-171°.
Picrate: Mp 208°.

[39111-57-4]

Bredereck, H. *et al, Chem. Ber.*, 1965, **98**, 3178 (*synth*)
U.S. Pat., 3 925 552, (1975) (*Fuveau*); *CA*, **84**, 180208q (*synth, pharmacol*)

1*H*-Pyrazolo[1,5-*a*]indole P-1-00155

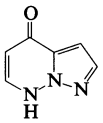


$C_{10}H_8N_2$ M 156.1
N-*Me:* [146979-87-5].
$C_{11}H_{10}N_2$ M 170.2 Pink cryst. (CH_2Cl_2/pentane). Mp 104°.

Shen, J.K. *et al, J.C.S. Perkin 1*, 1994, 1871 (*synth, pmr, cmr, uv*)

Pyrazolo[1,5-*b*]pyridazin-4(7*H*)-one, 9CI P-1-00156

[151554-78-8]



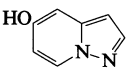
$C_6H_5N_3O$ M 135.1
No phys. props. descr.

Blake, A.J. *et al, Chem. Comm.*, 1993, 840 (*synth*)

Pyrazolo[1,5-*a*]pyridin-5-ol P-1-00157

5-Hydroxypyrazolo[1,5-a]pyridine

[156969-42-5]



$C_7H_6N_2O$ M 134.1
Pale yellow solid by subl. Mp 217° dec.

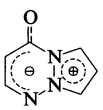
Ac: [156969-43-6].
$C_9H_8N_2O_2$ M 176.1 Pale yellow needles. Mp 67-67.5°.

Brown, R.F.C. *et al, Aust. J. Chem.*, 1994, **47**, 991 (*synth, uv, pmr, cmr*)

Pyrazolo[1,2-*a*][1,2,3]triazin-5-ium-4-olate P-1-00158

4-Hydroxypyrazolo[1,2-a][1,2,3]triazin-5-ium inner salt, 9CI

[151554-76-6]



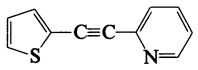
$C_6H_5N_3O$ M 135.1
Cryst.

Blake, A.J. *et al, Chem. Comm.*, 1993, 840 (*synth, cryst struct*)

(2-Pyridinyl)(2-thienyl) acetylene P-1-00159

2-(2-Thienylethynyl)pyridine, 9CI

[93297-80-4]



$C_{11}H_7NS$ M 185.2
Cryst. by subl. Mp 52-54°.

Novak, I. *et al, J.C.S. Perkin 2*, 1994, 1771 (*synth, uv, pmr, pe*)

(2-Pyridinyl)(3-thienyl) acetylene P-1-00160

2-(3-Thienylethynyl)pyridine, 9CI

[157798-74-8]

$C_{11}H_7NS$ M 185.2
Mp 56-58°.

Novak, I. *et al, J.C.S. Perkin 2*, 1994, 1771 (*synth, uv, pmr, pe*)

(3-Pyridinyl)(2-thienyl) acetylene P-1-00161

3-(2-Thienylethynyl)pyridine, 9CI

[157798-73-7]

$C_{11}H_7NS$ M 185.2
Mp 41-41.5°.

Novak, I. *et al, J.C.S. Perkin 2*, 1994, 1771 (*synth, uv, pmr, pe*)

(3-Pyridinyl)(3-thienyl) acetylene P-1-00162

3-(3-Thienylethynyl)pyridine, 9CI

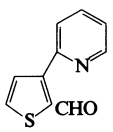
[157798-75-9]

$C_{11}H_7NS$ M 185.2
Mp 63.5-64°.

Novak, I. *et al, J.C.S. Perkin 2*, 1994, 1771 (*synth, uv, pmr, pe*)

3-(2-Pyridinyl)-2-thiophenecarboxaldehyde P-1-00163

2-Formyl-3-(2-pyridinyl)thiophene



$C_{10}H_7NOS$ M 189.2
Mp 72-74°.

Zhang, Y. *et al, J. Het. Chem.*, 1995, **32**, 435 (*synth, pmr, cmr*)

3-(3-Pyridinyl)-2-thiophenecarboxaldehyde, 9CI P-1-00164

2-Formyl-3-(3-pyridinyl)thiophene

[169701-91-1]

$C_{10}H_7NOS$ M 189.2
Mp 128-129.5°.

Zhang, Y. *et al, J. Het. Chem.*, 1995, **32**, 435 (*synth, pmr, cmr*)

3-(4-Pyridinyl)-2-thiophenecarboxaldehyde P-1-00165

2-Formyl-3-(4-pyridinyl)thiophene

$C_{10}H_7NOS$ M 189.2
Mp 77-80°.

Zhang, Y. *et al, J. Het. Chem.*, 1995, **32**, 435 (*synth, pmr, cmr*)

4-(3-Pyridinyl)-2-thiophenecarboxaldehyde P-1-00166

2-Formyl-4-(3-pyridinyl)thiophene

$C_{10}H_7NOS$ M 189.2
Mp 107-109°.

Zhang, Y. *et al, J. Het. Chem.*, 1995, **32**, 435 (*synth, pmr, cmr*)

4-(4-Pyridinyl)-2-thiophenecarboxaldehyde P-1-00167

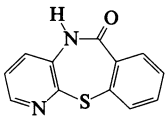
2-Formyl-4-(4-pyridinyl)thiophene

$C_{10}H_7NOS$ M 189.2
Mp 98-101.5°.

Zhang, Y. *et al, J. Het. Chem.*, 1995, **32**, 435 (*synth, pmr, cmr*)

Pyrido[2,3-*b*][1,4] benzothiazepin-6(5*H*)-one, 9CI P-1-00168

[106515-31-5]

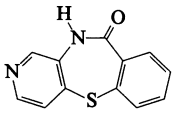


$C_{12}H_8N_2OS$ M 228.2
Solid. Mp 205-206°.

Liégeois, J.-F.F. *et al, J. Med. Chem.*, 1994, **37**, 519 (*synth*)

Pyrido[4,3-*b*][1,4] benzothiazepin-10(11*H*)-one, 9CI P-1-00169

[106515-32-6]

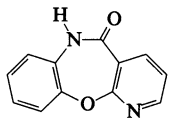


$C_{12}H_8N_2OS$ M 228.2
Solid. Mp 244-246°.

Liégeois, J.-F.F. *et al, J. Med. Chem.*, 1994, **37**, 519 (*synth, ir, pmr*)

Pyrido[2,3-*b*][1,5] benzoxazepin-5(6*H*)-one P-1-00170

[10189-46-5]

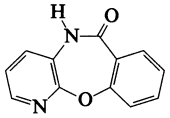


$C_{12}H_8N_2O_2$ M 212.2
Needles (dioxan or MeOH). Mp 260°.

Hoffman, C. *et al, Bull. Soc. Chim. Fr.*, 1966, 2316 (*synth*)

Pyrido[2,3-*b*][1,4]benzoxazepin-6(5*H*)-one, 9CI P-1-00171

[14470-90-7]



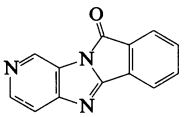
$C_{12}H_8N_2O_2$ M 212.2
Solid. Mp 268-269°.

Liégeois, J.-F.F. *et al, J. Med. Chem.*, 1994, **37**, 519 (*synth*)

10*H*-Pyrido[4′,3′:4,5] imidazo[2,1-*a*]isoindol-10-one, 9CI P-1-00172

Isoindolo[2,1-a]imidazo[5,4-c]pyridin-10-one

[158530-99-5]



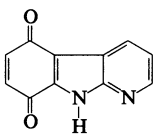
$C_{13}H_7N_3O$ M 221.2
Solid. Mp >200°.

Meegalla, S.K. *et al, J. Med. Chem.*, 1994, **37**, 3434 (*synth, ir, pmr, cmr*)

1*H*-Pyrido[2,3-*b*]indole-5,8-dione, 9CI P-1-00173

α-Carboline-6,9-quinone

[128040-59-5]



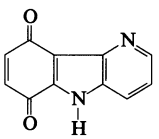
$C_{11}H_6N_2O_2$ M 198.1
Bright red cryst. ($CHCl_3$). Mp >200° dec.

Parrick, J. *et al, J. Chem. Res., Synop.*, 1990, **1**, 201 (*synth, ir, pmr, ms*)
Mehta, L.K. *et al, J.C.S. Perkin 1*, 1993, 1261 (*synth*)

5*H*-Pyrido[3,2-*b*]indole-6,9-dione P-1-00174

δ-Carboline-6,9-quinone

[151598-80-0]



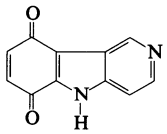
$C_{11}H_6N_2O_2$ M 198.1
Orange cryst. ($CHCl_3$).

Mehta, L.K. *et al, J.C.S. Perkin 1*, 1993, 1261 (*synth, ir, pmr, ms*)

5*H*-Pyrido[4,3-*b*]indole-6,9-dione P-1-00175

γ-Carboline-6,9-quinone

[151598-76-4]



$C_{11}H_6N_2O_2$ M 198.1

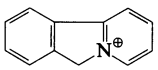
Dark red cryst. (MeOH/petrol). Mp >300° dec. >200°.

Mehta, L.K. *et al, J.C.S. Perkin 1*, 1993, 1261 (*synth, ir, pmr, ms*)

6*H*-Pyrido[2,1-*a*] isoindolium(1+), 9CI P-1-00176

6H-Benz[a]indolizinium

[13388-06-2]



$C_{12}H_{10}N^{\oplus}$ M 168.2 (ion)

Bromide: [13160-91-3].
$C_{12}H_{10}BrN$ M 248.1 Cryst. + $0.5H_2O$. Mp 207.5-209.5°. λ_{max} 256 (ε 4.14), 313 nm (4.02) in H_2O.

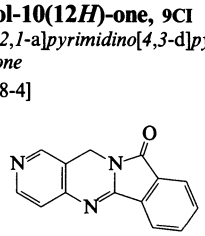
Perchlorate: [81123-84-4].
$C_{12}H_{10}ClNO_4$ M 267.6 Cryst.

Fozard, A. *et al, J.O.C.*, 1967, **32**, 2966 (*synth, uv*)
Romanov, N.N. *et al, Ukr. Khim. Zh.* (*Russ. edn.*), 1981, **47**, 1280; *CA*, **96**, 124505v (*synth*)
Kovtunenko, V.A. *et al, Ukr. Khim. Zh.* (*Russ. edn.*), 1985, **51**, 976; *CA*, **104**, 167711k (*struct*)

Pyrido[4′,3′:4,5]pyrimido[2,1-*a*]isoindol-10(12*H*)-one, 9CI P-1-00177

Isoindolo[2,1-a]pyrimidino[4,3-d]pyridin-10(12H)-one

[158530-98-4]



$C_{14}H_9N_3O$ M 235.2

Dark purple solid. Mp 254-256°.

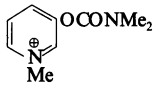
Meegalla, S.K. *et al, J. Med. Chem.*, 1994, **37**, 3434 (*synth, pmr, ir, cmr*)

Pyridostigmine(1+) P-1-00178

Updated Entry replacing P-0-04159

3-[[(Dimethylamino)carbonyl]oxy]-1-methylpyridinium, 9CI. 3-Hydroxy-1-methylpyridinium dimethylcarbamate, 8CI

[155-97-5]



$C_9H_{13}N_2O_2^{\oplus}$ M 181.2 (ion)

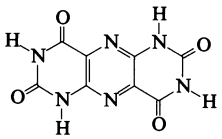
▶ UU5283000.

Bromide: [101-26-8]. ***Pyridostigmine bromide, BAN, USAN, INN, JAN.*** *Kalymin. Mestinon. Regonol. Ro 1-5130*
$C_9H_{13}BrN_2O_2$ M 261.1 Cholinergic agent. Prophylactic for military nerve agent poisoning. Used in treatment of myasthenia gravis. Hygroscopic cryst. (EtOH). Sol. H_2O. Mp 152-154°.

▶ Potential contact sensitiser. LD_{50} (rat, orl) 37.5 mg/kg. UU5270000.

Swiss Pat., 246 834, (1947); *CA*, **43**, 5050 (*synth*)
Millner, E.O. *et al, J. Med. Chem.*, 1974, **17**, 13 (*synth, pharmacol*)
Breyer-Pfaff, U. *et al, Clin. Pharmacol. Ther.* (*St. Louis*), 1985, **37**, 495 (*pharmacol*)
Inns, R.H. *et al, Clinical and Experimental Toxicology of Organophosphates and Carbamates*, (eds. Ballantyne, B., *et al*) Butterworth-Heinemann,Oxford, 1992, 602 (*use*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 1120.
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MDL600, PPI800.

2,4,7,9(1*H*,3*H*,6*H*,8*H*)-Pyrimido[4,5-*g*]pteridine-2,4,7,9(3*H*,8*H*)-tetrone P-1-00179



$C_8H_4N_6O_4$ M 248.1

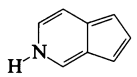
N,N′,N″,N‴-*Tetra-Me:* [7464-89-3]. *1,6-Dihydro-1,3,6,8-tetramethylpyrimido[4,5-g]pteridine-2,4,7,9(3H,8H)-tetrone, 9CI*
$C_{12}H_{12}N_6O_4$ M 304.2 Yellow prisms (DMF). Mp 358-360°.

Yoneda, F. *et al, Chem. Pharm. Bull.*, 1971, **19**, 1064 (*N-tetra-Me*)
Romerosa, A. *et al, Acta Cryst. C*, 1995, **51**, 1005 (*cryst struct, N-tetra-Me*)

2*H*-2-Pyrindine, 9CI, 8CI P-1-00180

Cyclopenta[c]pyridine

[270-58-6]



2H-form

C_8H_7N M 117.1

This compd. has not been reported. Investigated theoretically.

Treibs, W. *et al, Annalen*, 1962, **652**, 192.
Raimondi, M. *et al, Gazz. Chim. Ital.*, 1968, **98**, 433.
Evleth, E.M., *Theor. Chim. Acta*, 1970, **16**, 22.
Fabian, J., *Z. Phys. Chem.*, 1979, **260**, 81.

1*H*-Pyrrole-1-propanoic acid P-1-00181

[89059-06-3]

$C_7H_9NO_2$ M 139.1

Cryst. (Et_2O/petrol). Mp 62.5° (59-60°). $Bp_{0.4}$ 114°.

Me ester: [99233-38-2].
$C_8H_{11}NO_2$ M 153.1 Bp_{16} 114-115°.

Nitrile: [43036-06-2]. *1H-Pyrrole-1-propanenitrile, 9CI. 1-(2-Cyanoethyl)-1H-pyrrole*
$C_7H_8N_2$ M 120.1 Bp_{20} 84°.

[50463-83-7]

Braunholz, J.T. *et al, J.C.S.*, 1962, 4346 (*synth*)
Evans, D.L. *et al, J.O.C.*, 1979, **44**, 497 (*nitrile*)
Jefford, C.W. *et al, Helv. Chim. Acta*, 1983, **66**, 2666 (*synth*)

1*H*-Pyrrole-2-propanoic acid P-1-00182

$C_7H_9NO_2$ M 139.1

Small plates (C_6H_6/petrol). Mp 85-86°. $Bp_{0.5}$ 130-135°.

Me ester: [69917-80-2].
$C_8H_{11}NO_2$ M 153.1 Liq. Mp 8-11°. $Bp_{0.3}$ 75°.

[39319-38-5, 55490-37-4, 55490-38-5, 55490-39-6]

Kutscher, W. *et al, Hoppe Seyler's Z. Physiol. Chem.*, 1952, **289**, 229 (*synth*)
Harley-Mason, J., *J.C.S.*, 1952, 2433 (*synth*)
Cavalleri, B. *et al, Farmaco, Ed. Sci.*, 1975, **30**, 110 (*synth, derivs*)
Bates, H.A. *et al, J.A.C.S.*, 1979, **101**, 1259.
Bertschy, H. *et al, Angew. Chem., Int. Ed.*, 1990, **29**, 777 (*synth*)

1*H*-Pyrrole-3-propanoic acid P-1-00183

3-(3-Pyrrolyl)propionic acid

[134448-22-9]

$C_7H_9NO_2$ M 139.1

Amide: [152509-75-6]. *1H-Pyrrole-3-propanamide.* ***Cystamidin A***
$C_7H_{10}N_2O$ M 138.1 Prod. by *Streptomyces* sp. KP-1241. Calpain inhibitor. Powder. Mp 146-148°.

[107748-37-8, 150985-69-6]

Eur. Pat., 569 122, (1993); *CA*, **120**, 105131 (*Cystamidin A, isol, pmr, cmr, uv, ir*)
Hodges, L.M. *et al, J.O.C.*, 1993, **58**, 4788 (*Me ester*)

Pyrrolidine, 9CI, 8CI P-1-00184

Updated Entry replacing P-0-04275

Tetrahydropyrrole. Tetramethyleneimine. Azacyclopentane

[123-75-1]

C_4H_9N M 71.1

Present in tobacco and carrot leaves (*Daucus carota*) (Umbelliferae). Widely distributed in trace amts., presumably as bacterial decarboxylation prod. of proline. Manuf. by catalytic reaction of NH_3 with tetrahydrofuran or butanediol. Widely used org. base, used in the prep. of enamines. Reagent used in the ms detn. of the position of double bonds and of methyl branching in fatty acids. Liq. with odour resembling Piperidine, P-0-02980. Misc. H_2O. d_4^{20} 0.8618. Fp −63°. Bp 88.5-89°. pK_a 11.31 (25°). Fumes in air. Strongly alkaline.

▶ Highly flammable, fl. p. 3°. Skin, eye and respiratory tract irritant. LD_{50} (rat, orl) 300 mg/kg. UX9650000.

Hemipicrate: Dark-red cryst. Mp 163-164°.
Monopicrate: [1689-56-1].
Yellow needles (EtOH). Mp 112°.

N-*Ac:* [4030-18-6].
$C_6H_{11}NO$ M 113.1 Liq. Bp 224-225°.

N-*Benzoyl:* [3389-54-6].
$C_{11}H_{13}NO$ M 175.2 Liq. Bp_{20} 187°.

N-*Nitroso:* [930-55-2].
$C_4H_8N_2O$ M 100.1 Found in fried bacon, tobacco smoke. Oil. Bp 214°. n_D^{20} 1.4900.
▶ Exp. hepatocarcinogen. UY1575000.

N-*Me:* see *1-Methylpyrrolidine, M-0-04515*

N-*Et:* [7335-06-0].
$C_6H_{13}N$ M 99.1 Liq. Bp_{100} 50°.

N-*Propyl:* [7335-07-1].
$C_7H_{15}N$ M 113.2 Bp 130-135°.

N-*Butyl:* [767-10-2].
$C_8H_{17}N$ M 127.2 Liq. Bp 155-157°, Bp_{22} 55-56°. n_D^{20} 1.4400.
▶ UX9800000.

N-*Benzyl:* [29897-82-3].
$C_{11}H_{15}N$ M 161.2 Liq. Sol. EtOH, Et_2O. Bp 237°. Absorbs CO_2 and H_2O from the air.

N-*Ph:* see *1-Phenylpyrrolidine, P-0-02547*

N-*(2,4-Dinitrophenyl):* [14552-00-2].
Cryst. (cyclohexane/EtOAc). Mp 101.5-102.5°.

N-*Amino:* [16596-41-1]. *1-Aminopyrrolidine. 1-Pyrrolidinamine, 9CI*
$C_4H_{10}N_2$ M 86.1 Bp_{13} 28-30°.

N-*Amino, picrate:* Mp 165° dec.

N-*(2-Chloroethyl):* [7250-67-1].
$C_6H_{12}ClN$ M 133.6 Mp 169.5-173° (as hydrochloride). CAS no. refers to hydrochloride.
▶ UY0703150.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **1**, 557C, 623B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 353C, 355A, 398B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 442A, 443B, 481B (*ir*)
de Jong, M. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1930, **49**, 237 (*synth*)
Ochiai, E. *et al*, *Ber.*, 1934, **67**, 1017 (*derivs*)
Rink, M. *et al*, *Naturwissenschaften*, 1961, **48**, 51 (*N-amino*)
Duffield, A.M. *et al*, *J.A.C.S.*, 1965, **87**, 2920 (*ms*)
Wilshire, J.F.K., *Aust. J. Chem.*, 1966, **19**, 1935 (*deriv*)
Andersson, B.A. *et al*, *Lipids*, 1974, **9**, 185, 443; 1975, **10**, 215, 716 (*use*)
Hawthorne, D.G. *et al*, *Aust. J. Chem.*, 1976, **29**, 315 (*cmr*)
Ahmed, M.G. *et al*, *J.C.S. Perkin 2*, 1978, 372 (*cmr, derivs*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 428.
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, **A2**, 13 (*rev*)
Barbry, D. *et al*, *Magn. Reson. Chem.*, 1990, **28**, 560 (*cmr, N-15 nmr*)
Hunt, E.J. *et al*, *Carcinogenesis (London)*, 1991, **12**, 571 (*N-nitroso, bibl*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BSK250, NLP500, PPS500.
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 1090.

1-Pyrrolidinecarboxamide, 9CI P-1-00185

N-*Carbamoylpyrrolidine. 1-(Aminocarbonyl) pyrrolidine*

[4736-71-4]

$C_5H_{10}N_2O$ M 114.1
Metab. of the Mediterranean sponge *Aplysina (Verongia) cavernicola*. Cryst. (H_2O). Mp 148-152° (nat.), Mp 218° (synth.).

Reppe, W. *et al*, *Annalen*, 1955, **596**, 80 (*synth*)
D'Ambrosio, M. *et al*, *Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **83**, 309 (*isol, ir, pmr, cmr, ms*)

1-Pyrrolidinecarboxylic acid, 9CI P-1-00186

Tetramethylenecarbamic acid

$C_5H_9NO_2$ M 115.1

Me ester: [56475-80-0]. *1-Methoxycarbonylpyrrolidine*
$C_6H_{11}NO_2$ M 129.1 Liq. Bp_{13} 79-80°.

Et ester: [5470-26-8]. *1-Ethoxycarbonylpyrrolidine*
$C_7H_{13}NO_2$ M 143.1 Liq. Bp_3 61-62°.

Chloride: [1192-63-8]. *1-(Chlorocarbonyl) pyrrolidine*
C_5H_8ClNO M 133.5 Liq. Bp_{27} 115°.

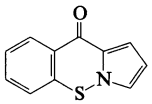
Amide: see *1-Pyrrolidinecarboxamide, P-1-00185*

Nitrile: [1530-88-7]. *1-Cyanopyrrolidine*
$C_5H_8N_2$ M 96.1 d 0.95. Bp_{10} 133°, $Bp_{1.8}$ 75-77°. n_D^{20} 1.4690.

Overman, L.E. *et al*, *J.A.C.S.*, 1980, **102**, 747 (*nitrile*)
Kita, Y. *et al*, *J.O.C.*, 1980, **45**, 4519 (*esters*)
Shono, T. *et al*, *Org. Synth.*, 1985, **63**, 206 (*Me ester*)
Raucher, S. *et al*, *Synth. Commun.*, 1985, **15**, 1025 (*Me ester*)
Hoshino, O. *et al*, *Synth. Commun.*, 1987, **17**, 1887 (*chloride*)

10*H*-Pyrrolo[1,2-*b*][1,2]benzothiazin-10-one P-1-00187

[153716-47-3]



$C_{11}H_7NOS$ M 201.2
Yellow-orange solid (EtOAc/hexane). Mp 100-102°.

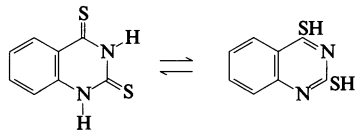
Bates, D.K. *et al*, *J.O.C.*, 1994, **59**, 8076 (*synth, ir, pmr, cmr*)

Q

2,4-Quinazolinedithiol Q-1-00001

2,4(1H,3H)-Quinazolinedithione, 9CI. 2,4-Dimercaptoquinazoline

[5993-69-1]



$C_8H_6N_2S_2$ M 194.2

Long yellow needles (*n*-butanol). Mp 335-338° dec. (313° dec.).

Di-NH-form

3N-Me: [16081-92-8].
$C_9H_8N_2S_2$ M 208.3 Cryst. Mp 290-296°.

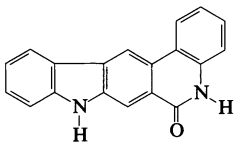
N,N′-*Di-Me:* [17489-72-4].
$C_{10}H_{10}N_2S_2$ M 222.3 Orange-yellow needles. Mp 267-268°.

Di-SH-form

S,S′-*Di-Me:* [48141-61-3]. *2,4-Bis(methylthio) quinazoline, 9CI*
$C_{10}H_{10}N_2S_2$ M 222.3 Solid. Mp 85°.

Elion, G.B. *et al, J.A.C.S.*, 1947, **69**, 2138 (*synth*)
Yale, H.L., *J.A.C.S.*, 1953, **75**, 675 (*synth*)
Taylor, E.C. *et al, Tetrahedron*, 1967, **23**, 891 (*synth*)
Wagner, G. *et al, Z. Chem.*, 1967, **7**, 339; 1969, **9**, 446 (*synth, derivs*)
Chern, J.-W. *et al, J. Med. Chem.*, 1993, **36**, 2196 (*synth, pmr, cmr*)

8*H*-Quino[3,4-*b*]carbazol-1(2*H*)-one Q-1-00002

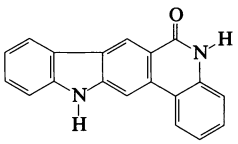


$C_{19}H_{12}N_2O$ M 284.3

Solid. Mp >350°.

Mohanakrishnan, A.K. *et al, J.O.C.*, 1995, **60**, 1939 (*synth, ir, pmr*)

8*H*-Quino[4,3-*b*]carbazol-1(2*H*)-one Q-1-00003



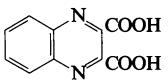
$C_{19}H_{12}N_2O$ M 284.3

Solid. Mp >350°.

Mohanakrishnan, A.K. *et al, J.O.C.*, 1995, **60**, 1939 (*synth, ir, pmr*)

2,3-Quinoxalinedicarboxylic acid Q-1-00004

[6924-99-8]



$C_{10}H_6N_2O_4$ M 218.1

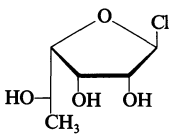
Dinitrile: [17132-92-2]. *2,3-Dicyanoquinoxaline*
$C_{10}H_4N_4$ M 180.1 Cryst. (EtOH). Mp 218°.

Rothkopf, H.W. *et al, Chem. Ber.*, 1975, **108**, 875.
Monge, A. *et al, J. Het. Chem.*, 1994, **31**, 1135.

R

Rhamnofuranosyl chloride R-1-00001

6-Deoxymannofuranosyl chloride, 9CI



$C_6H_{11}ClO_4$ M 182.6

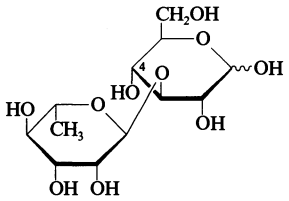
α-L-form

2,3-O-Isopropylidene, 5-tosyl: [32658-92-7].
$C_{16}H_{21}ClO_6S$ M 376.8 Syrup. Unstable at ambient temp.

Lerner, L.M. *et al, J.O.C.*, 1972, **37**, 477 (*isopropylidene deriv, pmr*)

3-*O*-α-L-Rhamnopyranosyl-D-glucose R-1-00002

3-O-(6-Deoxy-α-L-mannopyranosyl)-D-glucose, 9CI



$C_{12}H_{22}O_{10}$ M 326.3

4-O-(4-Hydroxy-E-cinnamoyl):
[104806-91-9]. ***Cistanoside I***
$C_{21}H_{28}O_{12}$ M 472.4 Isol. from *Cistanche salsa* (crude drug Cistanche herba). The crude drug is a tonic in oriental medicine. Hemihydrate. $[\alpha]_D^{20}$ −82.2 (c, 1.5 in MeOH).

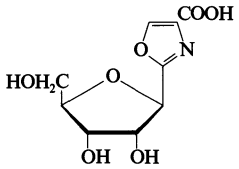
4-O-(3,4-Dihydroxy-E-cinnamoyl):
Cistanoside F
Isol. from *C. salsa*. Amorph. powder. $[\alpha]_D^{25}$ −83.5 (c, 0.9 in MeOH).

[97411-47-7]

Kobayashi, H. *et al, Chem. Pharm. Bull.*, 1985, **33**, 1452 (*Cistanoside F*)

Karasawa, H. *et al, Yakugaku Zasshi*, 1986, **106**, 562 (*Cistanoside I*)

2-β-D-Ribofuranosyl-4-oxazolecarboxylic acid, 9CI R-1-00003



$C_9H_{11}NO_7$ M 245.1

Amide: 2-β-D-Ribofuranosyl-4-oxazolecarboxamide, 9CI. Oxazofurin
$C_9H_{12}N_2O_6$ M 244.2 Oxygen analogue of tiazofurin and selenazofurin.

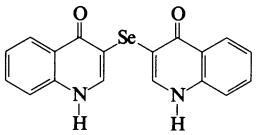
Me ester: [129149-88-8].
$C_{10}H_{13}NO_7$ M 259.2 Needles. Mp 114-115°.

[129149-89-9]

Franchetti, P. *et al, J. Med. Chem.*, 1990, **33**, 2849 (*synth, uv, pmr*)

S

3,3′-Selenobis[1,4-dihydro-4-quinolinone] S-1-00001



$C_{18}H_{12}N_2O_2Se$ M 367.2
Cryst. (EtOH/petrol) (as dihydrochloride). Mp >300° (dihydrochloride).

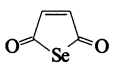
N,N′-*Di-Me:*
$C_{20}H_{16}N_2O_2Se$ M 395.3 Cryst. + 1 H_2O (H_2O). Mp 313°.

Löwe, W. *et al*, *J. Het. Chem.*, 1995, **32**, 271 (*synth, pmr*)

2,5-Selenophenedione, 9CI S-1-00002

1,4-Diselenomaleic acid cyclic anhydroselenide, 8CI

[26562-64-1]



$C_4H_2O_2Se$ M 161.0
Liq. $Bp_{0.5}$ 72°.

3,4-Dihydro: [26562-21-0]. *3,4-Dihydro-2,5-selenophenedione. 1,4-Diselenosuccinic acid cyclic anhydroselenide, 8CI*
$C_4H_4O_2Se$ M 163.0 Cryst. (EtOH/petrol). Mp 36°.

Morel, J. *et al*, *C. R. Hebd. Seances Acad. Sci. Ser. C*, 1970, **270**, 825 (*synth*)
Morel, J. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 3547 (*synth, ir, pmr, deriv*)

Spermic acid S-1-00003

N,N′-*1,4-Butanediylbis-β-alanine, 9CI. 4,9-Diazadodecanedioic acid.* N^1,N^4-*Bis(2-carboxyethyl)-1,4-butanediamine.* N,N′-*Tetramethylenedi-β-alanine. 1,4-Diaminobutane*-N,N′-*dipropanoic acid*

[14209-33-7]

$HOOCCH_2CH_2NH(CH_2)_4NHCH_2CH_2COOH$

$C_{10}H_{20}N_2O_4$ M 232.2
Isol. from bovine brain.

Di-Et ester: [87952-71-4].
$C_{14}H_{28}N_2O_4$ M 288.3 Powder (as hydrochloride). Mp 237-238° dec. (hydrochloride). CAS no. refers to hydrochloride.

[61345-82-2]

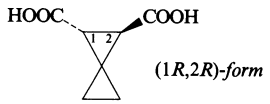
Imaoka, N. *et al*, *J. Neurochem.*, 1974, **22**, 859 (*isol*)
Tabor, H. *et al*, *Methods Enzymol.*, 1983, **94**, 418 (*rev, synth*)
Wasserman, H.H. *et al*, *Tetrahedron*, 1983, **39**, 2459 (*synth, ester*)
Ioannou, P.V., *Chem. Chron.*, 1991, **20**, 85 (*synth*)

Spiro[2.4]hepta-1,4,6-triene S-1-00004

C_7H_6 M 90.1

Billups, W.E. *et al*, *J.A.C.S.*, 1994, **116**, 6463 (*synth, pmr, cmr*)

1,2-Spiropentanedicarboxylic acid S-1-00005



(1*R*,2*R*)-*form*

$C_7H_8O_4$ M 156.1

(1R,2R)-form

Di-Me ester: [163380-56-1].
$C_9H_{12}O_4$ M 184.1 $[\alpha]_{546}$ −69 (c, 0.9 in CCl_4) (>99% ee).

(1RS,2RS)-form

(±)-trans-*form*

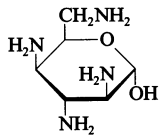
Di-Me ester: [163228-42-0].
Liq. $Bp_{0.3}$ 60° (Kugelrohr).

[163380-57-2]

Baldwin, J.E. *et al*, *J.O.C.*, 1995, **60**, 2635 (*synth, pmr*)

T

2,3,4,6-Tetraamino-2,3,4,6-tetradeoxyidose T-1-00001



$C_6H_{16}N_4O_2$ M 176.2

α-D-Pyranose-form

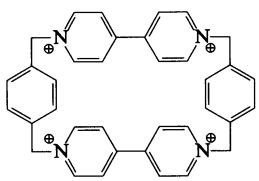
Me glycoside, 2N,3N,4N,6N-tetra-Ac: [17014-18-5].
$C_{15}H_{26}N_4O_6$ M 358.3 Cryst. (EtOH aq.). $[\alpha]_D^{21}$ +42 (c, 0.5 in H_2O). Dec. >260° without melting.

Ali, Y. *et al, Chem. Comm.*, 1967, 554 (*tetra-Ac*)
Ali, Y. *et al, J.C.S.(C)*, 1968, 1764 (*tetra-Ac, pmr*)

5,12,19,26-Tetraazoniaheptacyclo [24.2.2.2^{2,5}.2^{7,10}.2^{12,15}.2^{16,19}.2^{21,24}]tetraconta-2,4,7,9,12,14,16,18,21,23,26,28,29,31,33,35,37,39-octadecaene(4+), 9CI T-1-00002

*Cyclobis(paraquat-*p*-phenylene)*

[117271-76-8]



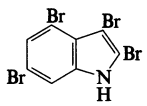
$C_{36}H_{32}N_4^{4\oplus}$ M 520.6 (ion)

Tetrakis(hexafluorophosphate): [117271-77-9].
$C_{36}H_{32}F_{24}N_4P_4$ M 1100.5 Solid (Me_2CO aq.). Mp >275°.

Anelli, P. *et al, J.A.C.S.*, 1992, **114**, 193 (*synth, cryst struct, pmr, cmr, ms*)
Cordova, E. *et al, J.O.C.*, 1995, **60**, 1033 (*use, bibl*)

2,3,4,6-Tetrabromo-1*H*-indole, 9CI T-1-00003

[128351-87-1]



$C_8H_3Br_4N$ M 432.7
Alkaloid from the Okinawan red alga *Laurencia brongniartii*. Cryst. (hexane/CCl_4). Mp 137-141°.

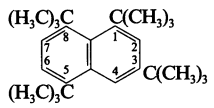
N-Ac:
$C_{10}H_5Br_4NO$ M 474.7 Mp 176-178°.

Tanaka, J. *et al, Tetrahedron*, 1989, **45**, 7301 (*isol, ir, pmr, ms, struct*)

1,3,5,8-Tetra-*tert*-butylnaphthalene T-1-00004

1,3,5,8-Tetrakis(1,1-dimethylethyl)naphthalene

[22550-43-2]



$C_{26}H_{40}$ M 352.6
Cryst. (MeOH). Mp 83-86°.

Franck, R.W. *et al, J.O.C.*, 1970, **35**, 3932.

1,3,6,8-Tetra-*tert*-butylnaphthalene T-1-00005

1,3,6,8-Tetrakis(1,1-dimethylethyl)naphthalene

[22495-86-9]

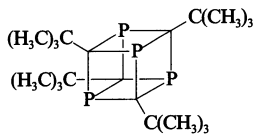
$C_{26}H_{40}$ M 352.6
Cryst. (MeOH). Mp 127-128°.

Franck, R.W. *et al, J.O.C.*, 1970, **35**, 3932.

1,3,5,7-Tetra-*tert*-butyl-1,3,5,7-tetraphosphacubane T-1-00006

2,4,6,8-Tetrakis(1,1-dimethylethyl)-1,3,5,7-tetraphosphapentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane

[121097-72-1]



$C_{20}H_{36}P_4$ M 400.3
Pale yellow cubes (pentane). Mp 241°. $Bp_{0.01}$ 155° (oven).

Monomethotriflate: Mp 200° dec.
Monoxide:
$C_{20}H_{36}OP_4$ M 416.3 Mp 264°. $Bp_{0.001}$ 200° (oven).

Monomethotetrafluoroborate:
$C_{21}H_{39}BF_4P_4$ M 502.2 Cryst. Mp 283° dec.

Wettling, T. *et al, Angew. Chem., Int. Ed.*, 1989, **28**, 1013 (*synth, ms, cmr, P-31 nmr, cryst struct*)
Gleiter, R. *et al, Chem. Ber.*, 1990, **123**, 757 (*pe, theory*)
Laali, K.K. *et al, J.O.C.*, 1993, **58**, 4105 (*derivs, synth, pmr, cmr, P-31 nmr*)

1,1,3,3-Tetra-*tert*-butyltriphosphine T-1-00007

1,1,3,3-Tetrakis(1,1-dimethylethyl)triphosphine

[118201-93-7]

$[(H_3C)_3C]_2P—PH—P[C(CH_3)_3]_2$

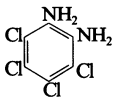
$C_{16}H_{37}P_3$ M 322.3
Needle-like cryst. (pentane at −30°). Mp 112°.

[118201-82-4, 137564-88-6]

Fritz, G. *et al, Z. Anorg. Allg. Chem.*, 1987, **552**, 18; 1987, **553**, 85; 1989, **570**, 54 (*synth, pmr, P-31 nmr*)
Scheer, M. *et al, Z. Anorg. Allg. Chem.*, 1991, **600**, 203; 1993, **619**, 1047 (*synth, P-31 nmr, salts*)

3,4,5,6-Tetrachloro-1,2-benzenediamine T-1-00008

*1,2-Diamino-3,4,5,6-tetrachlorobenzene. Tetrachloro-*o*-phenylenediamine*



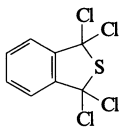
$C_6H_4Cl_4N_2$ M 245.9
Hydrochloride: Mp 212-214° dec.

Al Attar, A.F. *et al, Analyst (London)*, 1990, **115**, 1441 (*synth*)

1,1,3,3-Tetrachloro-1,3-dihydrobenzo[c]thiophene, 9CI T-1-00009

1,1,3,3-Tetrachlorothiophthalan

[13169-42-1]

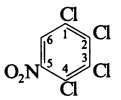


$C_8H_4Cl_4S$ M 273.9
Cryst. (hexane). Mp 111-112°.

Yagupolskii, L.M. *et al, Zh. Obshch. Khim.*, 1966, **36**, 1414; *J. Gen. Chem. USSR (Engl. Transl.)*, 1966, **36**, 1421 (*synth*)
Okuda, Y. *et al, J.O.C.*, 1991, **56**, 6024 (*synth, pmr*)

1,2,3,4-Tetrachloro-5-nitrobenzene, 9CI T-1-00010

[879-39-0]



$C_6HCl_4NO_2$ M 260.8
Needles (EtOH). Mp 66-67°.

Berckmans, V.S.F. *et al, Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1925, **44**, 851 (*synth*)
Suzuki, H. *et al, Synthesis*, 1994, 841 (*synth, ir, pmr, cmr, ms*)

1,2,3,5-Tetrachloro-4-nitrobenzene, 9CI T-1-00011

[3714-62-3]

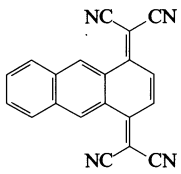
$C_6HCl_4NO_2$ M 260.8
Needles (EtOH). Mp 41-42° (38-40°).

Berckmans, V.S.F. *et al, Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1925, **44**, 851 (*synth*)
Suzuki, H. *et al, Synthesis*, 1994, 841 (*synth, ir, pmr, cmr, ms*)

11,11,12,12-Tetracyano-1,4-anthraquinodimethane T-1-00012

2,2'-(1,4-Anthracenediylidene) bispropanedinitrile, 9CI

[88068-06-8]



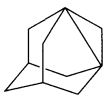
$C_{20}H_8N_4$ M 304.3
Red cryst. by subl. Mp >320° dec.

Yamaguchi, S. *et al, Chem. Lett.*, 1983, 1229 (*synth, pmr, ir, uv*)

Tetracyclo[3.3.1.1^{3,7}.0^{1,3}]decane T-1-00013

Tetrahydro-1H,4H-2,5:3a,6a-dimethanopentalene, 9CI. 1,3-Dehydroadamantane

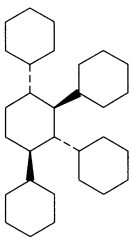
[24569-89-9]



$C_{10}H_{14}$ M 134.2
Solid by subl. Unstable, stored in a sealed tube under N_2.

Pincock, R.E. *et al, J.A.C.S.*, 1969, **91**, 4593 (*synth, ir, pmr*)
Bielmann, R. *et al, Helv. Chim. Acta*, 1982, **65**, 1728 (*synth, ir*)
Adcock, W. *et al, J.O.C.*, 1993, **58**, 7341 (*synth, cmr*)

1,2,3,4-Tetracyclohexylcyclohexane T-1-00014



(1*RS*,2*RS*,3*RS*,4*RS*)-*form*

$C_{30}H_{52}$ M 412.7

(***1RS,2RS,3RS,4RS*)-*form***
all-trans-*form*
No Mp given.

(***1RS,2RS,3RS,4SR*)-*form***
cis-trans-trans-*form*
No Mp given. Exists in twist-boat conformn.

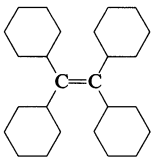
(***1RS,2SR,3SR,4RS*)-*form***
cis-trans-cis-*form*
Rectangular cryst. Mp 145°.

Columbus, I. *et al, J.A.C.S.*, 1994, **116**, 10306 (*synth, cmr, cryst struct, conformn*)

Tetracyclohexylethene T-1-00015

1,1',1'',1'''-(1,2-Ethenediylidene) tetrakiscyclohexane, 9CI

[155144-20-0]



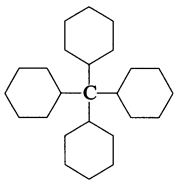
$C_{26}H_{44}$ M 356.6
Cryst. Mp 273-275°.

Columbus, I. *et al, J.O.C.*, 1994, **59**, 3402 (*synth, cryst struct, ir, cmr, pmr*)

Tetracyclohexylmethane T-1-00016

1,1',1'',1'''-Methanetetrayltetrakiscyclohexane, 9CI

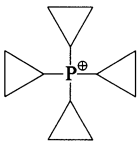
[1593-07-3]



$C_{25}H_{44}$ M 344.6
Cryst. ($CHCl_3$/EtOH). Mp 282° (270-272°).

Buell, G.R. *et al, J.O.C.*, 1965, **30**, 1662 (*synth, ir*)
Columbus, I. *et al, J.O.C.*, 1994, **59**, 8132 (*synth, pmr, cmr, conformn, cryst struct*)

Tetracyclopropylphosphonium(1+) T-1-00017



$C_{12}H_{20}P^{\oplus}$ M 195.2 (ion)

Chloride: [80095-65-4].
$C_{12}H_{20}ClP$ M 230.7 Cryst. (MeOH/EtOAc).

Schmidbaur, H. *et al, Chem. Ber.*, 1981, **114**, 3385 (*synth, pmr, P-31 nmr*)

2-Tetradecen-1-ol T-1-00018

$H_3C(CH_2)_{10}CH{=}CHCH_2OH$

$C_{14}H_{28}O$ M 212.3

(***E*)-*form*** [75039-86-0]
Liq. $Bp_{0.07}$ 105°.

[75039-85-9]

Doolittle, R.E., *Synthesis*, 1984, 730 (*synth, ir, pmr*)
Mordini, A. *et al, J.O.C.*, 1994, **59**, 4784 (*synth, pmr, cmr, ms*)

Tetradecylphosphonic acid T-1-00019

1-Tetradecanephosphonic acid

[4671-75-4]

$H_3C(CH_2)_{13}P(O)(OH)_2$

$C_{14}H_{31}O_3P$ M 278.3
Solid. Mp 97-98°.

Di-Et ester: [5191-09-3]. *Diethyl tetradecylphosphonate*
$C_{18}H_{39}O_3P$ M 334.4 Liq. Bp_3 200°.

Dibutyl ester: Dibutyl tetradecylphosphonate
$C_{22}H_{47}O_3P$ M 390.5 Liq. d_4^{25} 0.91. Bp_2 217-219°. n_D^{25} 1.4460.

Di-Ph ester: [16165-51-8]. *Diphenyl tetradecylphosphonate*
$C_{26}H_{39}O_3P$ M 430.5 Cryst. (pentane). Mp 41.5-42°. $Bp_{0.02}$ 197°.

[16693-58-6]

Kosolapoff, G.M., *J.A.C.S.*, 1945, **67**, 1180.
Laughton, R.G., *J.O.C.*, 1962, **27**, 3644 (*di-Ph ester*)

3,3,8,8-Tetraethynyl-1,4,6,9-decatetrayne, 9CI T-1-00020

[160651-50-3]

$(HC{\equiv}C)_3CC{\equiv}CC{\equiv}CC(C{\equiv}CH)_3$

$C_{18}H_6$ M 222.2
Off-white solid. Mp 151° dec.

Feldman, K.S. *et al, J.A.C.S.*, 1994, **116**, 9019.

2,2,2,3'-Tetrafluoroacetophenone, 8CI T-1-00021

2,2,2-Trifluoro-1-(3-fluorophenyl)ethanone, 9CI. 1-Fluoro-3-(trifluoroacetyl)benzene

[708-64-5]

$C_8H_4F_4O$ M 192.1
d 1.37. Bp_{50} 79°. n_D^{20} 1.4440.

Taft, R.W. *et al, J.A.C.S.*, 1963, **85**, 709 (*pmr*)
Liu, K.T. *et al, J. Phys. Org. Chem.*, 1989, **2**, 363 (*synth, O-17 nmr*)

2,2,2,4'-Tetrafluoroacetophenone T-1-00022

2,2,2-Trifluoro-1-(4-fluorophenyl)ethanone, 9CI. 4'-Fluoro-2,2,2-trifluoroacetophenone. 1-Fluoro-4-(trifluoroacetyl)benzene

[655-32-3]

$C_8H_4F_4O$ M 192.1
d 1.37. Mp 24-27°. Bp_{34} 66-67°. n_D^{20} 1.4480.

De Puy, C.H. *et al, J.O.C.*, 1974, **39**, 878 (*synth*)
Chong, J.M. *et al, J.O.C.*, 1991, **56**, 893 (*synth, pmr, cmr*)

2,2,3,3-Tetrafluoro-1,4-butanediol T-1-00023

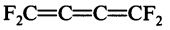
[425-61-6]

$HOCH_2CF_2CF_2CH_2OH$

$C_4H_6F_4O_2$ M 162.0
Cryst. (CCl_4/EtOAc). Mp 80.5-82°. pK_a 12.1 (13.7).

McBee, E.T., *J.A.C.S.*, 1952, **74**, 444.
Ward, R.B., *J.O.C.*, 1965, **30**, 3009.

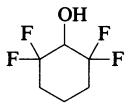
Tetrafluorobutatriene T-1-00024



C_4F_4 M 124.0
Bp 5°. Explodes when liquefied.

Martin, E.L. *et al, J.A.C.S.*, 1959, **81**, 5256.

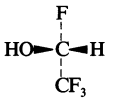
2,2,6,6-Tetrafluorocyclohexanol T-1-00025



$C_6H_8F_4O$ M 172.1
Mp 65-66°.

Duhamel, P. *et al, J.C.S. Perkin 1*, 1994, 2265 (*synth, pmr*)

1,2,2,2-Tetrafluoroethanol T-1-00026



(*R*)-*form*

$C_2H_2F_4O$ M 118.0

(R)-form

Me ether: [156700-90-2]. *1,1,1,2-Tetrafluoro-2-methoxyethane, 9CI*
$C_3H_4F_4O$ M 132.0 Intermed. in synth. of Desflurane, D-0-00462. Liq. Bp 38-39°. $[\alpha]_D^{25}$ +67 (neat) (97% ee).

Trichloromethyl ether:
$C_3HCl_3F_4O$ M 235.3 Liq. $[\alpha]_D^{25}$ +36 (c, 1 in $CHCl_3$). Cont. 10% of tetrachlorinated impurity.

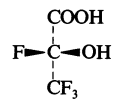
(±)-form

Me ether: Liq. Bp 36-38°.
Trichloromethyl ether: Liq. Bp 96-97°, Bp_{145} 44-47°.

[156700-89-9]

Ramig, K. *et al, Angew. Chem., Int. Ed.*, 1995, **34**, 222 (*synth, abs config*)
Rozov, L.A. *et al, J.O.C.*, 1995, **60**, 1319 (*Me ether, synth*)

2,3,3,3-Tetrafluoro-2-hydroxypropanoic acid T-1-00027



(*R*)-*form*

$C_3H_2F_4O_3$ M 162.0

(R)-form

Me ether: [156700-95-7]. *2,3,3,3-Tetrafluoro-2-methoxypropanoic acid*
$C_4H_4F_4O_3$ M 176.0 Liq. Bp_8 60-61°. $[\alpha]_D^{25}$ +24 (neat) (>99.9% ee).

Me ether, amide:
$C_4H_5F_4NO_2$ M 175.0 Cryst. (CH_2Cl_2). Mp 114°. $[\alpha]_D^{25}$ +33 (c, 1 in MeOH).

(±)-form

Me ether: [10186-64-8].
Liq. Bp_{13} 71.5-72.5°.

Me ether, Me ester: [10186-63-7].
$C_5H_6F_4O_3$ M 190.0 Liq. Bp_{21} 40-41°.

Me ether, chloride:
$C_4H_3ClF_4O_2$ M 194.5 Liq. Bp 78-80°.

Me ether, amide: [10186-65-9].
$C_4H_5F_4NO_2$ M 175.0 Cryst. (C_6H_6). Mp 109°.

Et ether: [10186-67-1]. *2-Ethoxy-2,3,3,3-tetrafluoropropanoic acid*
$C_5H_6F_4O_3$ M 190.0 Liq. Bp_{13} 83-84°.

Et ether, Et ester: [10186-66-0].
$C_7H_{10}F_4O_3$ M 218.1 Liq. Bp_{14} 50.5-51°.

Et ether, chloride:
$C_5H_5ClF_4O_2$ M 208.5 Liq. Bp_{773} 97°.

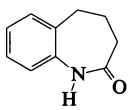
Et ether, amide: [10186-68-2].
$C_5H_7F_4NO_2$ M 189.1 Cryst. (CCl_4). Mp 82°.

[156700-86-6]

Sianesi, D. *et al, J.O.C.*, 1966, **31**, 2312 (*deriv, synth*)
Pasetti, A. *et al, Gazz. Chim. Ital.*, 1968, **98**, 277 (*deriv, synth*)
Muffler, H. *et al, J. Fluorine Chem.*, 1982, **21**, 107 (*chloride synth, pmr*)
Ramig, K. *et al, Angew. Chem., Int. Ed.*, 1995, **34**, 222 (*abs config*)
Rozov, L.A. *et al, J.O.C.*, 1995, **60**, 1319 (*Me ether, synth, resoln, pmr, F-19 nmr*)

1,3,4,5-Tetrahydro-2*H*-1-benzazepin-2-one, 9CI T-1-00028

[4424-80-0]

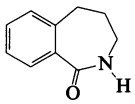


$C_{10}H_{11}NO$ M 161.2
Cryst. (EtOAc/hexane). Mp 141°.

Conley, R.T., *J.O.C.*, 1958, **23**, 1330.
Grunewald, G.L. *et al, J. Het. Chem.*, 1994, **31**, 1609 (*synth, pmr*)

2,3,4,5-Tetrahydro-1*H*-2-benzazepin-1-one, 9CI T-1-00029

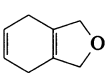
[6729-50-6]



$C_{10}H_{11}NO$ M 161.2
Cryst. ($CHCl_3$/hexane). Mp 130-131.5° (98-100°).

Gilman, N.W., *Synth. Commun.*, 1982, **12**, 373.
Grunewald, G.L. *et al, J. Het. Chem.*, 1994, **31**, 1609 (*synth, pmr, cmr*)

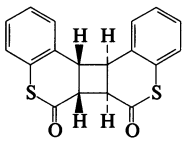
2,3,4,7-Tetrahydrobenzo[*c*]furan T-1-00030



$C_8H_{10}O$ M 122.1
Liq. Bp_{15} 150°.

Brown, D.S. *et al, J.C.S. Perkin 1*, 1995, 1137 (*synth, ir, pmr, cmr, ms*)

6*a*,6*b*,12*b*,12*c*-Tetrahydrocyclobuta[1,2-*c*:4,3-*c'*]di[1]benzothiopyran-6,7-dione T-1-00031



$C_{18}H_{12}O_2S_2$ M 324.4

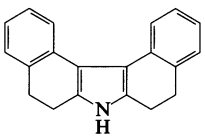
(6aα,6bβ,12bβ,12cα)-form

Photodimer of 2*H*-1-Benzothiopyran-2-one, B-0-01098. Cryst. (pentane). Mp 239-240°.

Kopf, J. *et al, Acta Cryst. C*, 1994, **50**, 1922 (*synth, cryst struct*)

6,7,8,9-Tetrahydro-5*H*-dibenzo[*c,g*]carbazole T-1-00032

[117766-87-7]



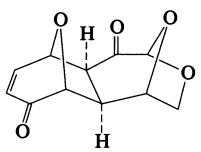
$C_{20}H_{17}N$ M 271.3
Mp 249-250°.

Katntcky, A.R. *et al, J. Het. Chem.*, 1988, **25**, 671.
Dimmock, J.R. *et al, J. Het. Chem.*, 1994, **31**, 1125 (*synth, cryst struct*)

5*a*,6,10,10*a*-Tetrahydro-1,4:6,10-diepoxy-2*H*-cyclohept[*d*]oxepin-5,9(1*H*,4*H*)dione, 9CI T-1-00033

5,13,14-Trioxatetracyclo[7.3.1.1^{3,6}.0^{2,8}]tetradec-10-ene-7,12-dione

[166241-44-7]



$C_{11}H_{10}O_5$ M 222.1
Pyrolysis prod. from Cellulose, C-0-00349.

Furneaux, R.H. *et al, J.C.S. Perkin 1*, 1984, 1923.
Gainsford, G.J. *et al, Acta Cryst. C*, 1995, **51**, 1369 (*cryst struct*)

1,2,3,4-Tetrahydro-2,8-dimethylnaphthalene T-1-00034

[25419-36-7]

$C_{12}H_{16}$ M 160.2

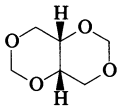
(±)-form

d^{20} 0.941. Bp 236°, Bp_{10} 102°.

Adv. Chem. Ser., 1955, **15**, 258 (***props***)

Tetrahydro[1,3]dioxino[5,4-*d*]-1,3-dioxin, 9CI T-1-00035

2,4,7,9-Tetraoxabicyclo[4.4.0]decane. 1,3,5,7-Tetraoxadecalin



(*S,S*)-*form*

$C_6H_{10}O_4$ M 146.1

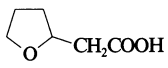
(***S,S*)-*form*** [75096-35-4]
(+)-cis-*form. 1,3:2,4-Di*-O-*methylene*-L-*threitol*
Mp 180-180.5°. $[\alpha]_D^{20}$ +10.71 (c, 0.11 in $CHCl_3$), $[\alpha]_D^{25}$ −4.1 (c, 2.1 in H_2O).

(***RS,SR*)-*form*** [54933-94-7]
trans-*form*
Needles (EtOAc/petrol). Mp 100°. *meso-*.

Lemieux, R.U. *et al, Can. J. Chem.*, 1963, **41**, 392 (*synth, pmr, cis*)
Jensen, R.B. *et al, Acta Chem. Scand., Ser. B*, 1975, **29**, 373 (*synth, trans-form*)
Burden, I.J. *et al, J.C.S. Perkin 1*, 1975, 666 (*synth, pmr, ms, trans-form*)
Noørskov, L. *et al, Acta Chem. Scand., Ser. B*, 1983, **37**, 133 (*conformn*)
Gras, J. *et al, Synth. Commun.*, 1992, **22**, 405 (*synth, pmr, trans*)

Tetrahydro-2-furanacetic acid T-1-00036

[2434-00-6]



$C_6H_{10}O_3$ M 130.1

(±)-***form*** [89261-69-8]
V. viscous oil or semisolid. Bp_{16} 144-146°, Bp_{11} 140°.

Me ester: [2018-85-1].
$C_7H_{12}O_3$ M 144.1 Liq. Bp_{19} 92°.

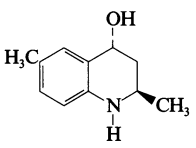
Et ester: [2434-02-8].
$C_8H_{14}O_3$ M 158.1 Oil.

Nitrile: [33414-62-9]. *2-(Cyanomethyl) tetrahydrofuran*
C_6H_9NO M 111.1 Liq. Bp_{13} 92.4°. n_D^{13} 1.4476.

Barger, G. *et al, J.C.S.*, 1937, 718 (*synth*)
Fissekis, J.D. *et al, J. Het. Chem.*, 1976, **13**, 929 (*Me ester, synth, pmr*)
Patrick, T.B. *et al, J.O.C.*, 1978, **43**, 1506 (*synth, ir, pmr*)

1,2,3,4-Tetrahydro-4-hydroxy-2,6-dimethylquinoline T-1-00037

1,2,3,4-Tetrahydro-2,6-dimethyl-4-quinolinol, 9CI



(2*RS*,4*RS*)-*form*

$C_{11}H_{15}NO$ M 177.2

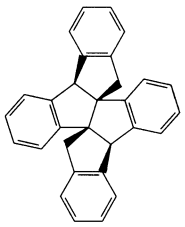
(***2RS,4RS*)-*form*** [63503-16-2]
(±)-trans-*form*
Cream powder. Mp 108-110° (100-102°).

(***2RS,4SR*)-*form*** [63503-15-1]
(±)-cis-*form*
Powder (EtOH). Mp 167-169°.

Crabb, T.A. *et al, J.C.S. Perkin 1*, 1994, 9 (*synth, pmr, bibl*)

4*b*,9,13*b*,18-Tetrahydroindeno[1,2-*a*]indeno[2′,1′:2,3]indeno[1,2-*b*]indene, 9CI T-1-00038

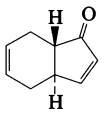
[155954-10-2]



$C_{30}H_{22}$ M 382.5
Needles ($CHCl_3$/hexane). Mp 200°.

Kuck, D. *et al, J.O.C.*, 1994, **59**, 2511 (*synth, ir, pmr, cmr, ms*)

3*a*,4,7,7*a*-Tetrahydro-1*H*-inden-1-one T-1-00039



$C_9H_{10}O$ M 134.1

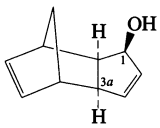
(***3aR,7aSR*)-*form***
(±)-trans-*form*
No phys. props. descr.

Nakatani, K. *et al, J.O.C.*, 1995, **60**, 2466 (*synth, pmr, cmr, ir, ms*)

3*a*,4,7,7*a*-Tetrahydro-4,7-methano-1*H*-inden-1-ol, 9CI T-1-00040

1-Hydroxydicyclopentadiene

[6814-80-8]



(1*R*,3*aS*,4*S*,7*R*,7*aS*)-*form*

$C_{10}H_{12}O$ M 148.2

(***1R,3aS,4S,7R,7aS*)-*form*** [123930-79-0]
Cryst. (hexane). Mp 72-72.5°. $[\alpha]_D^{25}$ +99.1 (c, 0.98 in $CHCl_3$).

(***1S,3aR,4R,7S,7aR*)-*form*** [105367-92-8]
Cryst. (hexane). Mp 72-72.5°. $[\alpha]_D^{25}$ −100.5 (c, 0.90 in $CHCl_3$).

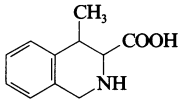
(***1RS,3aSR,4SR,7RS,7aSR*)-*form*** [88555-62-8]
Cryst. Mp 36-38°. Bp_7 106°.

Ac: [123848-89-5].
$C_{12}H_{14}O_2$ M 190.2 Oil. $Bp_{14.5}$ 118.5-120.5°.

Rosenblum, M., *J.A.C.S.*, 1957, **79**, 3179 (*synth, acetate*)
Nakagawa, K. *et al, Bull. Chem. Soc. Jpn.*, 1977, **50**, 2391 (*cmr*)
Mironov, V.A. *et al, Zh. Org. Khim.*, 1984, **20**, 69; *J. Org. Chem. USSR (Engl. Transl.)*, 1984, **20**, 61 (*synth*)
Takano, S. *et al, Chem. Comm.*, 1989, 271 (*resoln*)
Garland, R.B. *et al, J.O.C.*, 1990, **55**, 5854 (*synth*)
Shibuya, K., *Synth. Commun.*, 1994, **24**, 2923 (*synth*)

1,2,3,4-Tetrahydro-4-methyl-3-isoquinolinecarboxylic acid, 9CI T-1-00041

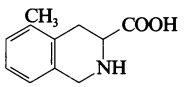
[106891-00-3]



$C_{11}H_{13}NO_2$ M 191.2
Intermed. for peptide synthesis. Cryst. (H_2O). Mp >260° dec.

Ger. Pat., 3 617 938, (1987); *CA*, **106**, 102109s (*synth*)
Lebl, M. *et al, Int. J. Pept. Protein Res.*, 1992, **40**, 148 (*synth*)

1,2,3,4-Tetrahydro-5-methyl-3-isoquinolinecarboxylic acid, 9CI T-1-00042



$C_{11}H_{13}NO_2$ M 191.2
Intermed. for peptide synthesis.

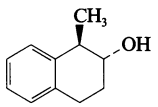
(±)-***form*** [151637-59-1]
Solid. Mp >280°.

Majer, P. *et al, Int. J. Pept. Protein Res.*, 1994, **43**, 62 (*synth, pmr*)

1,2,3,4-Tetrahydro-1-methyl-2-naphthol T-1-00043

1,2,3,4-Tetrahydro-1-methyl-2-naphthalenol, 9CI. 1-Methyl-2-tetralol

[86088-40-6]



(1*RS*,2*RS*)-*form*

$C_{11}H_{14}O$ M 162.2

(***1RS,2RS*)-*form*** [72182-04-8]
(±)-trans-*form*
Oil. $Bp_{0.2}$ 105-107°.

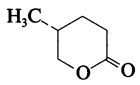
(***1RS,2SR*)-*form*** [91028-21-6]
(±)-cis-*form*
Oil. $Bp_{0.05}$ 73-74°.

McKusick, B.C. *et al, J.A.C.S.*, 1948, **70**, 2196 (*synth*)
Marshall, P.A. *et al, Aust. J. Chem.*, 1979, **32**, 1251 (*trans-form, synth, ir, pmr*)
Taylor, S.K. *et al, J.O.C.*, 1983, **48**, 2449; 1987, **52**, 425 (*cis-form, trans-form, ir, pmr*)
Schneider, H.-J. *et al, Org. Magn. Reson.*, 1984, **22**, 180 (*cmr*)

Tetrahydro-5-methyl-2*H*-pyran-2-one, 9CI T-1-00044

γ-Methyl-δ-valerolactone. 4-Methyl-5-pentanolide

[3123-98-6]



(*R*)-*form*

$C_6H_{10}O_2$ M 114.1

(***R*)-*form*** [2857-75-2]
Liq. Bp_7 101-102°. $[\alpha]_D^{20}$ +16.6 (c, 0.86 in $CHCl_3$) (>98% ee). n_D^{22} 1.4520.

(±)-***form*** [121961-94-2]
Liq. Bp_2 86°.

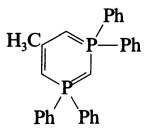
Brettle, R. *et al*, *J.C.S.*, 1962, 4836 (*synth*)
Millard, B.J., *Org. Mass Spectrom.*, 1968, **1**, 279 (*ms*)
Surzur, J.-M. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 653 (*synth, ir, pmr*)
Ozegowski, R. *et al*, *Annalen*, 1994, 1019 (*synth, pmr, cmr*)

1,1,3,3-Tetrahydro-5-methyl-1,1,3,3-tetraphenyl-1,3-diphosphorin, 9CI T-1-00045

Updated Entry replacing M-0-04674

5-Methyl-1,1,3,3-tetraphenyl-1λ⁵,3λ⁵-diphosphorine. 5-Methyl-1,1,3,3-tetraphenyl-1λ⁵,3λ⁵-diphosphabenzene. 5-Methyl-1,1,3,3-tetraphenyl-1λ⁵,3λ⁵-diphosphinin

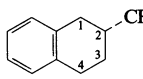
[125995-74-6]



$C_{29}H_{26}P_2$ M 436.4
Yellow cryst. (THF, −25°). Mp 115° dec. Planar, non-symmetric struct.

Schmidbaur, H. *et al*, *Angew. Chem., Int. Ed.*, 1990, **29**, 516 (*synth, pmr, cmr, P-31 nmr, cryst struct*)
Schmidbaur, H. *et al*, *Chem. Ber.*, 1991, **124**, 1525 (*synth, pmr, cmr, P-31 nmr, cryst struct*)

1,2,3,4-Tetrahydro-2-naphthaleneacetic acid T-1-00046



(*R*)-*form*

$C_{12}H_{14}O_2$ M 190.2

(***R*)-*form*** [130850-35-0]
Cryst. (diisopropyl ether). Mp 118-119°. $[\alpha]_D^{28}$ +79.8 (c, 0.96 in MeOH) (99.1% ee).

(***S*)-*form*** [130850-34-9]
Cryst. (diisopropyl ether). Mp 118-119°. $[\alpha]_D^{22}$ −80.1 (c, 1 in MeOH) (98.9% ee).

Chloride: [159011-43-5].
$C_{12}H_{13}ClO$ M 208.6 Oil. $Bp_{0.5}$ 98-100°.

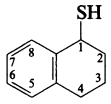
(±)-***form*** [147384-05-2]
Cryst. (EtOH aq.). Mp 85-87°.

Tanaka, Y. *et al*, *J. Med. Chem.*, 1994, **37**, 2071 (*synth, resoln, ir, pmr*)

1,2,3,4-Tetrahydro-1-naphthalenethiol, 9CI T-1-00047

1,2,3,4-Tetrahydro-1-mercaptonaphthalene. 1-Mercaptotetralin

[103324-34-1]



$C_{10}H_{12}S$ M 164.2

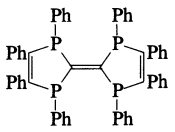
(±)-***form***
Liq. Bp_3 120°.

Nishio, T., *J.C.S. Perkin 1*, 1993, 1113 (*synth, ir, pmr, cmr*)

1,1′,3,3′-Tetrahydro-1,1′,3,3′,4,4′,5,5′-octaphenylbi-1,3-diphosphol-2-ylidene T-1-00048

2-(1,3-Dihydro-1,3,4,5-tetraphenyl-2H-1,3-diphosphol-2-ylidene)-2,3-dihydro-1,3,4,5-tetraphenyl-1H-1,3-diphosphole, 9CI

[114862-89-4]

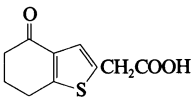


$C_{54}H_{40}P_4$ M 812.8

Maigrot, N. *et al*, *Angew. Chem., Int. Ed.*, 1988, **27**, 950 (*synth, ms, cmr, P-31 nmr*)

4,5,6,7-Tetrahydro-4-oxobenzo[*b*]thiophene-2-acetic acid, 9CI T-1-00049

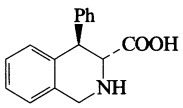
[158094-25-8]



$C_{10}H_{10}O_3S$ M 210.2
Cryst. (EtOAc/cyclohexane). Mp 130-132°.

Giardina, G. *et al*, *J. Med. Chem.*, 1994, **37**, 3482 (*synth, ir, pmr*)

1,2,3,4-Tetrahydro-4-phenyl-3-isoquinolinecarboxylic acid, 9CI T-1-00050



(3*R*,4*R*)-*form*

$C_{16}H_{15}NO_2$ M 253.3
Intermed. for peptide synthesis.

(***3R,4R*)-*form***
(−)-trans-*form*

Hydrochloride: Cryst. (6*M* HCl). Mp 263-266° dec. $[\alpha]_D$ −59.2 (c, 1 in MeOH).

(***3R,4S*)-*form***
(+)-cis-*form*

Hydrochloride: Cryst. (CH_3CN). Mp 255-258° dec. $[\alpha]_D$ +238.4 (c, 1 in MeOH).

(***3S,4R*)-*form***
(−)-cis-*form*

Hydrochloride: Cryst. (CH_3CN). Mp 256-258° dec. $[\alpha]_D$ −236.9 (c, 1 in MeOH).

(***3S,4S*)-*form***
(+)-trans-*form*

Hydrochloride: Cryst. (6*M* HCl). Mp 264-266° dec. $[\alpha]_D$ +58.8 (c, 1 in MeOH).

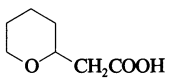
(***3RS,4RS*)-*form*** [153908-77-1]
(±)-trans-*form*
Needles (EtOH). Mp 160-162°.

N-*Me:* [153908-73-7].
$C_{17}H_{17}NO_2$ M 267.3 Needles (EtOH). Mp 174-178°.

U.K. Pat., 2 266 529, (1993); *CA*, **120**, 217313k (*synth, pmr*)
Goel, O.P. *et al*, *Synth. Commun.*, 1995, **25**, 49 (*synth, ir, pmr, cmr, ms*)

Tetrahydro-2*H*-pyran-2-acetic acid, 9CI T-1-00051

[13103-40-7]



$C_7H_{12}O_3$ M 144.1

(±)-***form*** [89261-76-7]
Cryst. (hexane). Mp 54-56°.

Et ester: [130821-87-3].
$C_9H_{16}O_3$ M 172.2 Liq. Bp_2 65-66°.

Chloride: [98431-12-0].
$C_7H_{11}ClO_2$ M 162.6 Liq. Bp_3 60-65°.

Amide:
$C_7H_{13}NO_2$ M 143.1 Cryst. (petrol). Mp 99-101°.

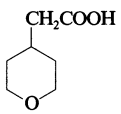
Nitrile: [89261-97-2]. *2-(Cyanomethyl) tetrahydropyran*
$C_7H_{11}NO$ M 125.1 Liq. Bp_{22} 110°.

[38786-78-6, 75394-84-2]

Zelinski, R.P. *et al*, *J.A.C.S.*, 1952, **74**, 1504 (*synth, chloride, amide*)
Maciejewski, L. *et al*, *Synth. Commun.*, 1988, **18**, 1757 (*synth, pmr, ms*)
Bunce, R.A. *et al*, *Synth. Commun.*, 1993, **23**, 1009 (*Et ester*)
Ragoussis, V. *et al*, *Synthesis*, 1993, 84 (*synth*)

Tetrahydro-2*H*-pyran-4-acetic acid, 9CI T-1-00052

[85064-61-5]

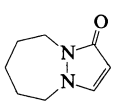


$C_7H_{12}O_3$ M 144.1
Cryst. solid. Mp 61-62°.

Ghosh, A.K. *et al*, *J. Med. Chem.*, 1993, **36**, 2300 (*synth*)

6,7,8,9-Tetrahydro-1*H*,5*H*-pyrazolo[1,2-*a*][1,2]diazepin-1-one, 9CI T-1-00053

[55781-91-4]



$C_8H_{12}N_2O$ M 152.1

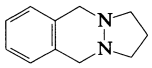
Hygroscopic cryst. (CH_2Cl_2/CCl_4). Mp 84°.

Hydrochloride: [66190-52-1].
Cryst. (MeOH or 1-propanol). Mp 175°, Mp 200-202°.

Sucrow, W. *et al*, *Chem. Ber.*, 1978, **111**, 780 (*synth, ir, uv, pmr, cmr*)
Arán, V.J. *et al*, *Annalen*, 1995, 817 (*synth*)

2,3,5,10-Tetrahydro-1*H*-pyrazolo[1,2-*b*]phthalazine T-1-00054

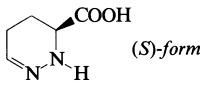
[28689-97-6]



$C_{11}H_{14}N_2$ M 174.2
Mp 70-72°. Bp_5 122°.

Nakamura, A. *et al*, *Chem. Pharm. Bull.*, 1970, **18**, 1526 (*synth, pmr*)

2,3,4,5-Tetrahydro-3-pyridazinecarboxylic acid, 9CI T-1-00055



$C_5H_8N_2O_2$ M 128.1

(S)-form [152094-16-1]

Trifluoroacetate salt: [152094-25-2].
$[\alpha]_D^{20}$ +62 (c, 0.3 in MeOH).

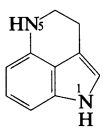
Me ester: [138323-06-5].
$C_6H_{10}N_2O_2$ M 142.1 Syrup. $[\alpha]_D^{20}$ +139 (c, 0.8 in MeOH).

[145022-62-4]

Nakamura, Y. *et al*, *Chem. Lett.*, 1991, 1953 (*synth, pmr*)
Aspinall, I.H. *et al*, *Chem. Comm.*, 1993, 1179 (*synth*)

1,3,4,5-Tetrahydropyrrolo[4,3,2-*de*]quinoline, 9CI T-1-00056

[5712-14-1]



$C_{10}H_{10}N_2$ M 158.2
Prisms (Et_2O/hexane). Mp 135-136° (130-131°).

1-Me:
$C_{11}H_{12}N_2$ M 172.2 Cryst. (MeOH/EtOAc) (as hydrochloride). Mp 220-235° dec. (hydrochloride).

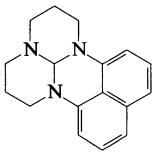
5-Me:
$C_{11}H_{12}N_2$ M 172.2 Mp 121-123°.

Hester, J.B., *J.O.C.*, 1964, **29**, 1159 (*synth, uv*)
Somei, M. *et al*, *Heterocycles*, 1991, **32**, 443; 1993, **36**, 2783 (*synth, ir, pmr*)
Roué, N. *et al*, *Synth. Commun.*, 1995, **25**, 681 (*synth, ir, uv, ms, pmr, cmr*)

2,3,5,6-Tetrahydro-1*H*,4*H*,12c*H*-3*a*,6*a*,12*b*-triazaperylene, 9CI T-1-00057

3a,6a,12b-Triaza-1,2,3,3a,4,5,6,6a,12b,12c-decahydroperylene

[166041-25-4]



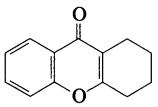
$C_{17}H_{19}N_3$ M 265.3
Cryst.

Baradarani, M.M. *et al*, *Acta Cryst. C*, 1995, **51**, 1345 (*synth, cryst struct*)

1,2,3,4-Tetrahydroxanthone T-1-00058

1,2,3,4-Tetrahydro-9H-xanthen-9-one, 9CI

[3123-22-6]



$C_{13}H_{12}O_2$ M 200.2
Needles (MeOH aq.); prisms (hexane). Mp 93-94° (91-92°), Mp 103-104° (dimorph.).

Hall, H.I. *et al*, *J.C.S.*, 1933, 232 (*synth*)
Miyano, M., *J.A.C.S.*, 1965, **87**, 3958 (*synth*)
Matsui, M. *et al*, *Agric. Biol. Chem.*, 1966, **30**, 1145 (*synth, ir*)
Paquette, L.A. *et al*, *J.O.C.*, 1966, **31**, 1232 (*synth*)
Watanabe, T. *et al*, *Chem. Pharm. Bull.*, 1977, **25**, 2778 (*synth, uv, pmr, ms*)
Singh, S.P. *et al*, *Synth. Commun.*, 1994, **24**, 2637 (*synth*)

1,4,5,8-Tetrahydroxyanthraquinone T-1-00059

1,4,5,8-Tetrahydroxy-9,10-anthracenedione, 9CI

[81-60-7]

$C_{14}H_8O_6$ M 272.2
Bronze needles. Mp >300° dec.

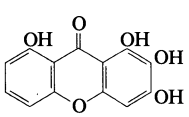
Tetra-Ac:
$C_{22}H_{16}O_{10}$ M 440.3 Yellow needles (AcOH). Mp 281-282°.

Tetra-Me ether: [63229-37-8]. *1,4,5,8-Tetramethoxyanthraquinone*
$C_{18}H_{16}O_6$ M 328.3 Orange leaflets (AcOH). Mp 327-329° (317°).

Fischer, O. *et al*, *J. Prakt. Chem.*, 1912, **86**, 297 (*synth, tetra-Ac, tetra-Me ether*)
Marshall, P.G., *J.C.S.*, 1937, 254 (*synth, tetra-Ac*)
Allen, C.F.H. *et al*, *J.O.C.*, 1941, **6**, 732 (*synth, tetra-Ac*)
Brockmann, H. *et al*, *Chem. Ber.*, 1965, **98**, 3145 (*uv*)
Quast, H. *et al*, *Chem. Ber.*, 1986, **119**, 1016 (*tetra-Me ether*)

1,2,3,8-Tetrahydroxyxanthone T-1-00060

1,2,3,8-Tetrahydroxy-9H-xanthen-9-one, 9CI



$C_{13}H_8O_6$ M 260.2

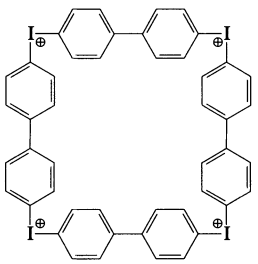
2-Me ether: [93929-99-8]. *1,3,8-Trihydroxy-2-methoxyxanthone*
$C_{14}H_{10}O_6$ M 274.2 Constit. of *Centaurium linarifolium*. Pale yellow cryst. (Me_2CO). Mp 262-264°.

1,2-Di-Me ether: [34211-52-4]. *3,8-Dihydroxy-1,2-dimethylxanthone*
$C_{15}H_{12}O_6$ M 288.2 Constit. of *Bonnetia dinizii, Calophyllum trapezifolium, Centaurium linarifolium* and *Polygala nyikensis*. Yellow powder. Mp 207-208°.

1,8-Di-Me ether, 2,3-methylene ether: [150921-43-0]. *1,8-Dimethoxy-2,3-methylenedioxyxanthone*
$C_{16}H_{12}O_6$ M 300.2 Constit. of the roots of *Polygala nyikensis*. Yellow powder. Mp 207-208°.

Parra, M. *et al*, *J. Nat. Prod.*, 1984, **47**, 868 (*isol, derivs*)
Vijayalakshmi, J. *et al*, *Acta Cryst. C*, 1987, **43**, 2108 (*cryst struct, deriv*)
Marston, A. *et al*, *Phytochemistry*, 1993, **33**, 809 (*isol, pmr, cmr*)

6,15,24,33-Tetraiodonianonacyclo-[32.2.2.2^{2,5}.2^{7,10}.2^{11,14}.2^{16,19}.2^{20,23}.2^{25,28}.2^{29,32}]dopentaconta-2,4,7,9,11,13,16,18,20,22,25,27,29,31,34,36,37,39,41,43,45,47,49,51-tetracosaene, 9CI T-1-00061



$C_{48}H_{32}I_4^{4\oplus}$ M 1116.3 (ion)

Tetrakis(trifluoromethanesulfonate): [152842-78-9].
$C_{52}H_{32}F_{12}I_4O_{12}S_4$ M 1712.6 Cryst. ($MeOH/Et_2O$). Mp 274-276° dec.

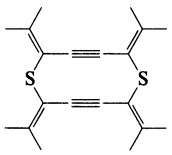
Tetrakis(tetraphenylborate): [152842-79-0].
$C_{144}H_{112}B_4I_4$ M 2393.3 Cryst. Spar. sol. common solvs. Mp 235-240° dec.

Tetrachloride: [152842-80-3].
$C_{48}H_{32}Cl_4I_4$ M 1258.2 Solid. Insol. all common solvs. Mp 200-205° dec.

Tetraiodide: [152842-81-4].
$C_{48}H_{32}I_8$ M 1624.0 Solid. Spar. sol. in common solvs. Mp 155-160° dec.

Stang, P.J. *et al*, *J.A.C.S.*, 1993, **115**, 9808 (*synth, ir, pmr, cmr, ms*)

2,5,7,10-Tetraisopropylidene-1,6-dithia-3,8-cyclodecadiyne T-1-00062



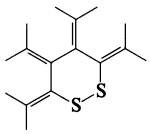
$C_{20}H_{24}S_2$ M 328.5
Cryst. (CH_2Cl_2 at −30°).

Gleiter, R. *et al, Angew. Chem., Int. Ed.*, 1994, **33**, 1270 (*synth, cryst struct*)

Tetraisopropylidene-1,2-dithiane T-1-00063

2,3,5,6-Tetrakis(1-methylethylidene)-1,2-dithiane, 9CI. 1,2-Dithia[6]radialene

[100671-37-2]



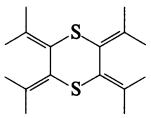
$C_{16}H_{24}S_2$ M 280.4
Mp 97.5-99.5°.

Ando, W. *et al, Tet. Lett.*, 1981, **22**, 4819 (*synth, cmr*)

Tetraisopropylidene-1,4-dithiane T-1-00064

3,4,5,6-Tetrakis(1-methylethylidene)-1,4-dithiane, 9CI. 1,4-Dithia[6]radialene

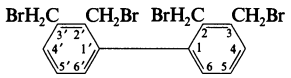
[100671-36-1]



$C_{16}H_{24}S_2$ M 280.4
Mp 99.5-100°.

Ando, W. *et al, Tet. Lett.*, 1981, **22**, 4819 (*synth, cmr, cryst struct*)
Gleiter, R. *et al, Angew. Chem., Int. Ed.*, 1994, **33**, 1270 (*synth*)

2,2′,3,3′-Tetrakis(bromomethyl)biphenyl T-1-00065



$C_{16}H_{14}Br_4$ M 525.9
Cryst. ($CHCl_3$). Mp 130-131°.

Grochowski, J. *et al, Annalen*, 1995, 1123 (*synth, ir, pmr, ms*)

2,2′,6,6′-Tetrakis(bromomethyl)biphenyl T-1-00066

[69551-56-0]

$C_{16}H_{14}Br_4$ M 525.9
Cryst. (propanol or petrol/C_6H_6). Mp 172-173.5° (167.5-168°).

Pelchowicz, Z. *et al, CA*, 1955, **49**, 1687i (*synth*)
Mislow, K. *et al, J.A.C.S.*, 1964, **86**, 1710 (*synth*)

3,3′,4,4′-Tetrakis(bromomethyl)biphenyl T-1-00067

[151331-25-8]

$C_{16}H_{14}Br_4$ M 525.9
Cryst. ($CHCl_3$). Mp 163-164°.

Jamrozik, J. *et al, J. Prakt. Chem.*, 1993, **335**, 482 (*synth, ir, pmr, cmr, ms*)

3,3′,5,5′-Tetrakis(bromomethyl)biphenyl biphenyl T-1-00068

[42601-58-1]

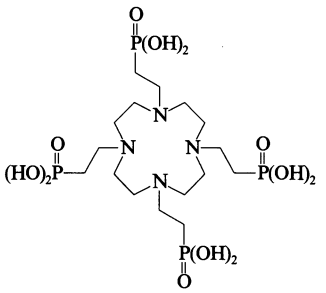
$C_{16}H_{14}Br_4$ M 525.9
Needles (C_6H_6/petrol); platelets (MeCN). Mp 208-210°.

Vögtle, F. *et al, Chem.-Ztg.*, 1973, **97**, 385 (*synth, pmr*)

1,4,7,10-Tetrakis[2-(dihydroxyphosphinyl)ethyl]-1,4,7,10-tetraazacyclododecane T-1-00069

[1,4,7,10-Tetraazacyclotetradecane-1,4,7,10-tetrayltetra-2,1-ethanediyl]tetrakisphosphonic acid, 9CI

[107145-38-0]



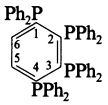
$C_{16}H_{40}N_4O_{12}P_4$ M 604.4
Complexone. Solid + $1H_2O$. Mp 268° dec.

Polikarpov, Yu.M. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1989, 2112; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1989, 1945 (*synth, complexes*)

1,2,3,4-Tetrakis(diphenylphosphino)benzene T-1-00070

1,2,3,4-Benzenetetrayltetrakis[diphenylphosphine], 9CI

[123739-97-9]



$C_{54}H_{42}P_4$ M 814.8
Yellow solid. Mp 235-239°.

McFarlane, H.C.E. *et al, Polyhedron*, 1988, **7**, 1875 (*synth, P-31 nmr*)

1,2,3,5-Tetrakis(diphenylphosphino)benzene T-1-00071

1,2,3,5-Benzenetetrayltetrakis[diphenylphosphine], 9CI

[123739-98-0]

$C_{54}H_{42}P_4$ M 814.8
Pale yellow solid. Mp 191-192°.

McFarlane, H.C.E. *et al, Polyhedron*, 1988, **7**, 1875 (*synth, P-31 nmr*)

1,2,4,5-Tetrakis(diphenylphosphino)benzene T-1-00072

1,2,4,5-Benzenetetrayltetrakis[diphenylphosphine], 9CI

[123739-99-1]

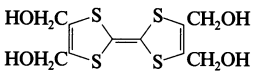
$C_{54}H_{42}P_4$ M 814.8
Ligand for Ni, Pd and Pt poly-complexes. Cryst. (MeOH/$CHCl_3$). Mp 271-273°.

McFarlane, H.C.E. *et al, Polyhedron*, 1988, **7**, 1875 (*synth, P-31 nmr*)
Wang, P.-W. *et al, Inorg. Chem.*, 1994, **33**, 2938 (*complexes*)

2,3,6,7-Tetrakis(hydroxymethyl)tetrathiafulvalene T-1-00073

2-[4,5-Bis(hydroxymethyl)-1,3-dithiol-2-ylidene]-1,3-dithiole-4,5-dimethanol, 9CI

[122301-05-7]



$C_{10}H_{12}O_4S_4$ M 324.4
Yellow-orange powder. Mp 190° dec.

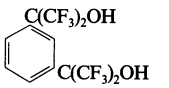
Tetra-Ac: [159223-16-2].
$C_{18}H_{20}O_8S_4$ M 492.6 Orange needles (hexane/CH_2Cl_2). Mp 131°.

Fox, M.A. *et al, J.O.C.*, 1994, **59**, 6519 (*synth, pmr, cmr, ir*)

α,α,α′α′-Tetrakis(trifluoromethyl)-1,3-benzenedimethanol, 9CI T-1-00074

α,α,α′,α′-Tetrakis(trifluoromethyl)-m-xylene-α,α′-diol, 8CI. 1,3-Bis(2-hydroxyhexafluoro-2-propyl)benzene

[802-93-7]



$C_{12}H_6F_{12}O_2$ M 410.1
Liq. d 1.66. Bp 209°, Bp_{24} 107-108°. n_D^{20} 1.3870.

DMSO complex (1:1): [89780-05-2].
Cryst. ($CHCl_3$). Mp 87°.
Di-Ac: [125757-14-4].
$C_{16}H_{10}F_{12}O_4$ M 494.2 Mp 80-82°.

Farah, B.S. *et al, J.O.C.*, 1965, **30**, 998 (*synth, pmr*)
Sepiol, J. *et al, J. Fluorine Chem.*, 1984, **24**, 61 (*synth, ir, pmr, F-19 nmr*)
Soulen, R.J. *et al, J. Fluorine Chem.*, 1989, **44**, 195 (*synth, pmr, Ac*)

Tetrakis(trifluoromethyl) diphosphine, 9CI, 8CI T-1-00075

[2714-60-5]

$(F_3C)_2P—P(CF_3)_2$

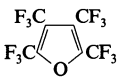
$C_4F_{12}P_2$ M 337.9
Stable liq. Mp 83-84°. P—P bond cleaved by I_2 or Br_2 at 280°.

Bennett, F.W. *et al*, *J.C.S.*, 1953, 1565 (*synth, ir*)
Cavell, R.G. *et al*, *Inorg. Chem.*, 1968, **7**, 690 (*ms*)
Kang, D.-K. *et al*, *Org. Magn. Reson.*, 1971, **3**, 101 (*F-19 nmr*)
Witt, J.D. *et al*, *Inorg. Chem.*, 1973, **12**, 811 (*ir, Raman*)
Bürger, H. *et al*, *Z. Anorg. Allg. Chem.*, 1973, **396**, 199 (*ir, Raman*)
Cowley, A.H. *et al*, *J.A.C.S.*, 1974, **96**, 2648, 3666 (*pe*)
Hodges, H.L. *et al*, *Inorg. Chem.*, 1975, **14**, 599 (*ed*)
Troy, D. *et al*, *Bull. Soc. Chim. Fr.*, (Part 1), 1979, 241 (*complexes*)
Grobe, J. *et al*, *J. Organomet. Chem.*, 1985, **280**, 331 (*complexes*)
Phillips, I.G. *et al*, *Inorg. Chem.*, 1988, **27**, 4038 (*props*)

Tetrakis(trifluoromethyl)furan T-1-00076

Perfluorotetramethylfuran

[67705-05-9]



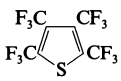
$C_8F_{12}O$ M 340.0
Bp 104-105°.

Boriack, C.J. *et al*, *Tet. Lett.*, 1978, 1015 (*synth, ir, uv*)
Kobayashi, Y. *et al*, *Tet. Lett.*, 1978, 1019 (*synth*)
Chambers, R.D. *et al*, *J.C.S. Perkin 1*, 1979, 214; 1994, 3119 (*synth*)

Tetrakis(trifluoromethyl) thiophene T-1-00077

Perfluorotetramethylthiophene

[651-93-4]



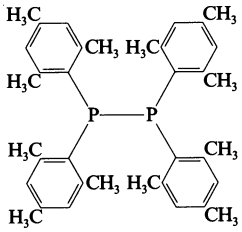
$C_8F_{12}S$ M 356.1
Liq. Mp 5°. Bp 134-135°. n_D^{25} 1.3540.

Krespan, C.G., *J.A.C.S.*, 1961, **83**, 3434 (*synth, uv*)
Briscoe, M.W. *et al*, *J.C.S. Perkin 1*, 1994, 3119 (*synth*)

Tetrakis(2,4,6-trimethylphenyl)diphosphine, 9CI T-1-00078

Tetramesityldiphosphine, 8CI

[23897-19-0]



$C_{36}H_{44}P_2$ M 538.6
Cryst. ($EtOH/C_6H_6$). Mp 210-215° dec.

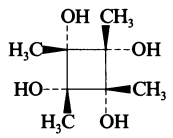
1-Oxide: [23921-55-3].
$C_{36}H_{44}OP_2$ M 554.6 Solid. Mp 205-208°.

1,2-Dioxide: [23897-21-4].
$C_{36}H_{44}O_2P_2$ M 570.6 Cryst. (2-butanone). Mp 188-190°.

Stepanov, B.I. *et al*, *Zh. Obshch. Khim.*, 1969, **39**, 1544; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1969, **39**, 1514 (*synth, ir, uv*)
Baxter, S.G. *et al*, *J.A.C.S.*, 1981, **103**, 1699 (*pmr, cryst struct*)
Goldwhite, H. *et al*, *J. Organomet. Chem.*, 1986, **310**, 21 (*synth*)

1,2,3,4-Tetramethyl-1,2,3,4-cyclobutanetetrol, 9CI T-1-00079

[117972-46-0]



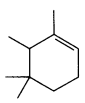
$C_8H_{16}O_4$ M 176.2

Kahle, C.F., *Diss. Abstr. Int., B*, 1988, **48**, 1981 (*synth*)
Olmstead, M.M. *et al*, *Acta Cryst. C*, 1992, **48**, 1902 (*cryst struct*)

1,5,5,6-Tetramethylcyclohexene, 9CI, 8CI T-1-00080

Cyclodihydromyrcene

[3757-05-9]

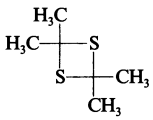


$C_{10}H_{18}$ M 138.2
(±)-*form*
Bp 171-172°, Bp_{12} 48°.

Ohloff, G., *Annalen*, 1959, **627**, 79 (*synth, ir*)
Naves, Y.R., *Helv. Chim. Acta*, 1964, **47**, 1833 (*synth, ir*)

2,2,4,4-Tetramethyl-1,3-dithietane T-1-00081

[31443-08-0]

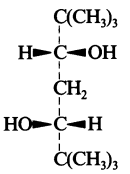


$C_6H_{12}S_2$ M 148.2
Needles (hexane). Mp 77-78°.

S,S,S′,S′-Tetraoxide: [82599-61-9].
$C_6H_{12}O_4S_2$ M 212.2 Fine white cryst. (DMF). Mp 270-274° dec.

Kohrman, R.E. *et al*, *J.O.C.*, 1971, **36**, 3971 (*synth, ir, uv, pmr, ms*)
Nishio, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 2253 (*synth, uv, ms*)
Block, E. *et al*, *J.A.C.S.*, 1982, **104**, 3119 (*tetraoxide, synth, ir, pmr*)
Frasch, M. *et al*, *Chem. Ber.*, 1993, **126**, 537 (*tetraoxide*)

2,2,6,6-Tetramethyl-3,5-heptanediol T-1-00082



(*3RS,5RS*)-*form*

$C_{11}H_{24}O_2$ M 188.3
(***3RS,5RS***)-***form*** [36402-58-1]
(±)-*form*
Fibre-like cryst. (hexane). Mp 178° (174°).
(***3RS,5SR***)-***form*** [36402-57-0]
meso-*form*
Needles by subl. Mp 101°.

Dale, J., *J.C.S.*, 1961, 910 (*synth*)
Cazaux, L. *et al*, *Bull. Soc. Chim. Fr.*, 1972, 773 (*synth, ir, pmr*)
Suzuki, I. *et al*, *J.A.C.S.*, 1993, **115**, 10139 (*synth, ir, pmr*)

2,2,6,6-Tetramethyl-3-heptene, 9CI T-1-00083

$(H_3C)_3CCH_2CH{=}CHC(CH_3)_3$

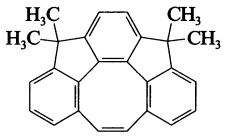
$C_{11}H_{22}$ M 154.2
(***E***)-***form*** [126029-24-1]
Liq. Bp_{85} 80-82°.
[126029-25-2]

Whitmore, F.C. *et al*, *J.A.C.S.*, 1941, **63**, 643 (*synth*)
Herberg, C. *et al*, *Annalen*, 1995, 515 (*synth, pmr*)

1,1,14,14-Tetramethyl-10,11-methano-1*H*-benzo[5,6]cycloocta[1,2,3,4-*def*]fluorene, 9CI T-1-00084

1,1-Dimethyl-10,11-propane-2,2-diylidene-1H-benzo[5,6]cycloocta[1,2,3,4-def]fluorene

[106865-76-3]



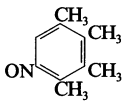
$C_{26}H_{22}$ M 334.4
Light yellow needles (EtOH). Mp 215-217°.

Hou, X.L. *et al*, *J.A.C.S.*, 1987, **109**, 1868 (*synth, pmr, uv*)
Felder, P. *et al*, *Helv. Chim. Acta*, 1991, **74**, 644 (*struct*)

1,2,3,4-Tetramethyl-5-nitrosobenzene T-1-00085

Nitrosoprehnitene

[158815-56-6]



$C_{10}H_{13}NO$ M 163.2
Green cryst. (MeOH). Mp 69-71°.

Smith, I.L. *et al*, *J.A.C.S.*, 1935, **57**, 2460 (*synth*)
Bosch, E. *et al*, *J.O.C.*, 1994, **59**, 5573 (*synth, ir, pmr, cmr*)

3,3,6,6-Tetramethyl-1,4,7-octatriyne, 9CI T-1-00086

[159148-55-7]

$HC{\equiv}CC(CH_3)_2C{\equiv}CC(CH_3)_2C{\equiv}CH$

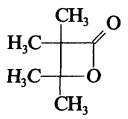
$C_{12}H_{14}$ M 158.2
Cryst. Mp 38-41°. Bp_{15} 62-64°.

Scott, L.T. *et al*, *J.A.C.S.*, 1994, **116**, 10275 (*synth, pmr, cmr, ms*)

3,3,4,4-Tetramethyl-2-oxetanone T-1-00087

Tetramethyl-β-propionolactone

[10008-69-2]



$C_7H_{12}O_2$ M 128.1
Solid. Mp 129-130°.

Adam, W. *et al*, *Synthesis*, 1972, 616 (*synth, ir, pmr*)
Schick, H. *et al*, *J.O.C.*, 1994, **59**, 3161 (*synth, ir, pmr, cmr*)

Tetramethyltellurium, 9CI T-1-00088

[123311-08-0]

$TeMe_4$

$C_4H_{12}Te$ M 187.7
Yellow-orange liq. Stable under Ar in the dark at r.t. Pyrophoric in air.

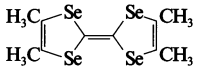
▶ Has exploded in air.

Gedridge, R.W. *et al*, *Organometallics*, 1989, **8**, 2817 (*synth, pmr, cmr, Te-125 nmr, ir, uv, Raman*)
Fowler, J.E. *et al*, *J.A.C.S.*, 1994, **116**, 9596 (*struct*)

Tetramethyltetraselenafulvalene T-1-00089

2-(4,5-Dimethyl-1,3-diselenol-2-ylidene)-4,5-dimethyl-1,3-diselenole, 9CI. TMTSF

[55259-49-9]



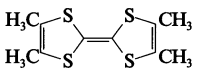
$C_{10}H_{12}Se_4$ M 448.0
Forms salts which are superconductive 'organic metals'. Violet needles. Mp >250°.

Bechgaard, K. *et al*, *Chem. Comm.*, 1974, 937 (*synth, uv*)
Andersen, J.R. *et al*, *Org. Mass Spectrom.*, 1978, **13**, 121 (*ms*)
Moradpour, A. *et al*, *J.O.C.*, 1983, **48**, 388 (*synth*)
Meneghetti, M. *et al*, *J. Chem. Phys.*, 1984, **80**, 6210 (*ir, Raman*)
Williams, J.M. *et al*, *Adv. Inorg. Chem. Radiochem.*, 1985, **29**, 249 (*rev*)

Tetramethyltetrathiafulvalene T-1-00090

2-(4,5-Dimethyl-1,3-dithiol-2-ylidene)-4,5-dimethyl-1,3-dithiole, 9CI. Tetramethyl-1,3-dithiol-2-ylidene. TMTTF

[50708-37-7]



$C_{10}H_{12}S_4$ M 260.4
Forms radical cation salts of high conductivity. Salmon-coloured needles (MeCN). Mp 244.5-245° (240.5-241°).

Ferraris, J.P. *et al*, *Tet. Lett.*, 1973, 2553 (*synth, ir, pmr*)
Wudl, F. *et al*, *J.O.C.*, 1977, **42**, 768 (*synth, uv, pmr, ir*)
Andersen, J.R. *et al*, *Org. Mass Spectrom.*, 1978, **13**, 121 (*ms*)
Le Costumer, G. *et al*, *Chem. Comm.*, 1980, 38 (*synth*)
Fabre, J.M. *et al*, *Bull. Soc. Chim. Fr.*, 1987, 823 (*synth, pmr*)

1,1,3,3-Tetramethyl-2-(trifluoromethyl)triphosphine, 9CI T-1-00091

[19307-60-9]

$(Me_2P)_2PCF_3$

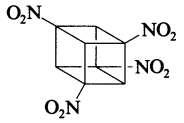
$C_5H_{12}F_3P_3$ M 222.0
Liq. at −5°. Bp 220° (est.). V.p. 1 mm at 24°.

Cowley, A.H. *et al*, *J.A.C.S.*, 1967, **89**, 5990; 1969, **91**, 6609 (*synth, uv, pmr, F-19 nmr, props*)
Avens, L.R. *et al*, *Inorg. Chem.*, 1989, **28**, 200, 205 (*synth, F-19 and P-31 nmr*)

1,3,5,7-Tetranitrocubane T-1-00092

1,3,5,7-Tetranitropentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane, 9CI

[99393-55-2]



$C_8H_4N_4O_8$ M 284.1
Solid. Mp 270° dec.

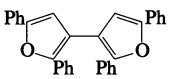
▶ Potentially explosive.

Eaton, P.E. *et al*, *J.A.C.S.*, 1993, **115**, 10195 (*synth, ir, pmr, cmr, cryst struct, haz*)

2,2′,5,5′-Tetraphenyl-3,3′-bifuran, 9CI T-1-00093

3,3′-Bis(2,5-diphenylfuran)

[52107-61-6]

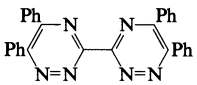


$C_{32}H_{22}O_2$ M 438.5
Yellow-white cryst. (EtOH or Me_2CO). Mp 195-196°.

Lutz, R.E. *et al*, *J.A.C.S.*, 1935, **57**, 1947 (*synth*)
Barba, F. *et al*, *J.O.C.*, 1993, **58**, 7685 (*synth, ir, pmr, ms, cmr*)

5,5′,6,6′-Tetraphenyl-3,3′-bi-1,2,4-triazine, 9CI T-1-00094

[93372-16-8]



$C_{30}H_{20}N_6$ M 464.5
Yellow cryst. (AcOH or toluene). Mp 297° dec., Mp 219-222°. Crimson soln. in H_2SO_4.

Laakso, P.V. *et al*, *Tetrahedron*, 1957, **1**, 103 (*synth*)
Breu, J. *et al*, *Acta Cryst. C*, 1993, **49**, 1541 (*cryst struct*)

1,1,2,4-Tetraphenyl-1-buten-3-yne T-1-00095

[21979-82-8]

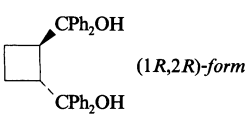
$Ph_2C{=}CPhC{\equiv}CPh$

$C_{28}H_{20}$ M 356.4
Cryst. (EtOH). Mp 136°.

Melloni, G. *et al*, *Chem. Comm.*, 1968, 1505 (*synth, ir, uv, pmr*)
Marcuzzi, F. *et al*, *J.C.S. Perkin 1*, 1993, 2957 (*synth*)

α,α,α′,α′-Tetraphenyl-1,2-cyclobutanedimethanol T-1-00096

1,2-Bis(hydroxydiphenylmethyl)cyclobutane



(1*R*,2*R*)-*form*

$C_{30}H_{28}O_2$ M 420.5

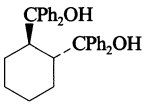
(1R,2R)-form
(−)-trans-*form*
Needles. Mp 174-175.5°. $[\alpha]_D^{29}$ −59 (c, 0.5 in Me_2CO). Racemate also known.

(1S,2S)-form
(+)-trans-*form*
Cryst. Mp 174-175.5° (170-171°). $[\alpha]_D^{20}$ +57.9 (c, 0.54 in Me_2CO).

Kipping, F.B. *et al*, *J.C.S.*, 1957, 3246 (*synth*)
Ito, Y.N. *et al*, *Helv. Chim. Acta*, 1994, **77**, 2071 (*synth, cryst struct*)

α,α,α′,α′-Tetraphenyl-1,2-cyclohexanedimethanol T-1-00097

1,2-Bis(hydroxydiphenylmethyl)cyclohexane



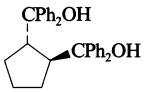
$C_{32}H_{32}O_2$ M 448.6

(1R,2R)-form [17351-17-6]
(+)-trans-*form*
Cryst. (hexane/EtOAc). Mp 189-190°. $[\alpha]_D^{20}$ +131 (c, 1.05 in Me_2CO) (>98% ee).

Ito, Y.N. *et al*, *Helv. Chim. Acta*, 1994, **77**, 2071 (*synth, ir, pmr, cryst struct*)

α,α,α′,α′-Tetraphenyl-1,2-cyclopentanedimethanol T-1-00098

1,2-Bis(hydroxydiphenylmethyl)cyclopentane



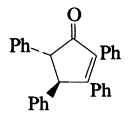
$C_{31}H_{30}O_2$ M 434.5

(1S,2S)-form
(+)-trans-*form*
Syrup. $[\alpha]_D^{20}$ +17.8 (c, 1.16 in $CHCl_3$).

Ito, Y.N. *et al*, *Helv. Chim. Acta*, 1994, **77**, 2071 (*synth, ir, pmr*)

2,3,4,5-Tetraphenyl-2-cyclopenten-1-one T-1-00099

[7317-52-4]



(3*RS*,4*RS*)-*form*

$C_{29}H_{22}O$ M 386.4

(3RS,4RS)-form [6177-94-2]
(±)-trans-*form*
Cryst. (EtOH). Mp 163°. Yellowish-green soln. in H_2SO_4.

(3RS,4SR)-form [15718-95-3]
(±)-cis-*form*
Cryst. (EtOH/cyclohexane). Mp 127-128°.

Dilthey, W. *et al*, *J. Prakt. Chem.*, 1930, **128**, 149; 1933, **139**, 1; 1937, **149**, 183 (*synth*)
Sonntag, N.O.V. *et al*, *J.A.C.S.*, 1953, **75**, 2283 (*synth*)
Rio, G. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 3774 (*synth, ir, pmr, uv*)
Harlow, R.L. *et al*, *Cryst. Struct. Commun.*, 1977, **6**, 695 (*cryst struct*)
Yuki, T. *et al*, *J.O.C.*, 1993, **58**, 4497 (*synth, pmr, cmr, ir*)

1,1,6,6-Tetraphenyl-2,4-hexadiyne-1,6-diol, 9CI T-1-00100

[20583-04-4]

$Ph_2C(OH)C{\equiv}CC{\equiv}CC(OH)Ph_2$

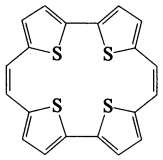
$C_{30}H_{22}O_2$ M 414.5
Versatile host for crystalline inclusion complexes. Has been used for example in isoln. of caffeine from tea, cholesterol from gallstones. Cryst. (C_6H_6/petrol). Mp 150-151°.

Armitage, J.B. *et al*, *J.C.S.*, 1951, 44 (*synth*)
Ried, W. *et al*, *Chem. Ber.*, 1963, **96**, 1226 (*synth*)
Toda, F., *Top. Curr. Chem.*, 1987, **140**, 43.
Segawa, M. *et al*, *Chem. Lett.*, 1988, 1755 (*use*)

Tetrathia[20]annulene[2,0,2,0] T-1-00101

21,22,23,24-Tetrathiapentacyclo[16.2.1.1^{2,5}.1^{8,11}.1^{12,15}]tetracosa-1,3,5,7,9,11,13,15,17,19-decaene, 9CI. Tetrathiaporphycene

[153580-77-9]



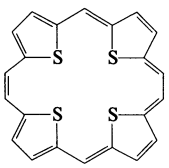
$C_{20}H_{12}S_4$ M 380.5
Yellow cryst. Mp 148-150°.

Hu, Z. *et al*, *J.O.C.*, 1994, **59**, 8071 (*synth, pmr, cmr, uv, ms*)

Tetrathia[22]annulene[2,1,2,1] T-1-00102

23,24,25,26-Tetrathiapentacyclo[18.2.1.1^{3,6}.1^{9,12}.1^{14,17}]hexacosa-1,3,5,7,9,11,13,15,17,19,21-undecaene

[156339-60-5]



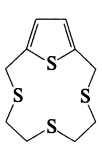
$C_{22}H_{14}S_4$ M 406.6
Black cryst. Mp >270°.

Hu, Z. *et al*, *J.O.C.*, 1994, **59**, 8071 (*synth, pmr, cmr, uv, ms*)

3,6,9,14-Tetrathiabicyclo[9.2.1]tetradeca-11,13-diene T-1-00103

2,5,8-Trithia[9](2,5)thiophenophane

[60147-18-4]



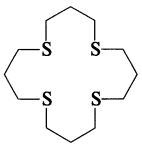
$C_{10}H_{14}S_4$ M 262.4
Needles (C_6H_6). Mp 125-127°, Mp 151-153°.

Weker, E. *et al*, *Annalen*, 1976, 891 (*synth, pmr, complexes*)
Lucas, C.R. *et al*, *Can. J. Chem.*, 1988, **66**, 1506 (*synth, cryst struct, cmr*)

1,5,9,13-Tetrathiacyclohexadecane, 9CI T-1-00104

16-Ane-S_4

[295-91-0]

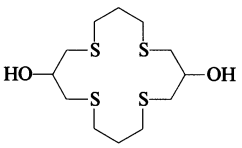


$C_{12}H_{24}S_4$ M 296.5
Potential ligand for transition metals. Mp 57-58°. Subl.$_{0.01}$ 100°.

Meadow, J.R. *et al*, *J.A.C.S.*, 1934, **56**, 2177 (*synth*)
Yoshida, T. *et al*, *Pure Appl. Chem.*, 1990, **62**, 1127 (*rev*)
Durrant, M.C. *et al*, *Chem. Ind.* (*London*), 1991, 474 (*synth, pmr*)
Setzer, W.N. *et al*, *Inorg. Chem.*, 1991, **30**, 3652 (*complexes*)
Blake, A.J. *et al*, *Acta Cryst. B*, 1993, **49**, 773 (*cryst struct*)

1,5,9,13-Tetrathiacyclohexadecane-3,11-diol, 9CI T-1-00105

[109909-33-3]



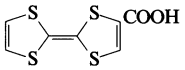
$C_{12}H_{24}O_2S_4$ M 328.5
Mp 89-91°. No synth. appears to have been publ.

Aldrich Library of FT-IR Spectra, 1st edn., **1**, 272D.
Nour, E.M. *et al*, *Bull. Soc. Chim. Fr.*, 1989, 727.
Wee, G. *et al*, *J.A.C.S.*, 1991, **113**, 6538.

Tetrathiafulvalenecarboxylic acid T-1-00106

2-(1,3-Dithiol-2-ylidene)-1,3-dithiole-4-carboxylic acid, 9CI. 2-Carboxytetrathiafulvalene

[63822-38-8]



$C_7H_4O_2S_4$ M 248.3
Used in the study of electrically conducting charge-transfer salts. Red needles (C_6H_6). Mp 182-184° (178°).

Me ester: [67361-89-1].
$C_8H_6O_2S_4$ M 262.3 Red powder (hexane). Mp 114° (102-104°).

Et ester: [63822-39-9].
$C_9H_8O_2S_4$ M 276.4 Red cryst. (MeOH). Mp 79.5-80.5°.

Green, D.C., *J.O.C.*, 1979, **44**, 1476 (*synth, Et ester, ir, pmr, uv*)
Kreitsberga, Ya.N. *et al*, *Khim. Geterotsikl. Soedin.*, 1984, 1630; *Chem. Heterocycl. Compd.* (*Engl. Transl.*), 1984, 1342 (*synth, Me ester, ir, pmr, uv*)
Fabre, J.-M. *et al*, *Makromol. Chem.*, 1989, **190**, 2747 (*synth*)
Fabre, J.-M. *et al*, *Bull. Soc. Chim. Belg.*, 1992, **101**, 741 (*cmr, pmr, Me ester*)
Garín, J. *et al*, *Synthesis*, 1994, 489 (*synth, pmr*)

1,2,3-Thiadiazole-4-carboxaldehyde T-1-00107

4-Formyl-1,2,3-thiadiazole

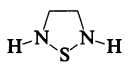
[27643-15-8]

$C_3H_2N_2OS$ M 114.1
Cryst. Mp 86-87°.

Lee, F.T. *et al*, *J. Het. Chem.*, 1970, **7**, 415 (*synth, ir, pmr*)
L'abbé, G. *et al*, *J. Het. Chem.*, 1993, **30**, 301 (*N-15 nmr*)

1,2,5-Thiadiazolidine T-1-00108

Tetrahydro-1,2,5-thiadiazole



$C_2H_6N_2S$ M 90.1

S,S-*Dioxide:* [5823-51-8].
$C_2H_6N_2O_2S$ M 122.1 Cryst. (EtOAc/hexane). Mp 53-54.5°.

N-*Me*, S,S-*dioxide:*
$C_3H_8N_2O_2S$ M 136.1 Oil. $Bp_{0.08}$ 145-155°.

N-tert-*Butyl*, S,S-*dioxide:*
$C_6H_{14}N_2O_2S$ M 178.2 Cryst. Mp 95-97°.

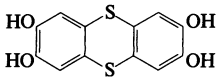
N,N′-*Di*-tert-*butyl*, S,S-*dioxide:*
$C_{10}H_{22}N_2O_2S$ M 234.3 Cryst. Mp 121-123°.

Preiss, M., *Chem. Ber.*, 1978, **111**, 1915 (*synth, derivs, ir, pmr*)
Castro, J.L. *et al*, *J. Med. Chem.*, 1994, **37**, 3023 (*synth, pmr*)

2,3,7,8-Thianthrenetetrol T-1-00109

2,3,7,8-Tetrahydroxythianthrene

[24066-96-4]



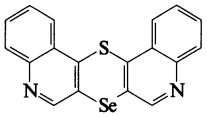
$C_{12}H_8O_4S_2$ M 280.3
Mp 288-289°.

Tetra-Me ether: [41079-73-6]. *2,3,7,8-Tetramethoxythianthrene*
$C_{16}H_{16}O_4S_2$ M 336.4 Cryst. (EtOH). Mp 183-184° (176°).

Weiss, T. *et al*, *Annalen*, 1978, 785 (*deriv*)
Nishiyama, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1994, **67**, 2333 (*synth*)

[1,4]Thiaselenino[3,2-*c*:5,6-*c*′]diquinoline, 9CI T-1-00110

[162469-49-0]



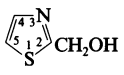
$C_{18}H_{10}N_2SSe$ M 365.3
Beige cryst. + ½ H_2O (EtOH). Mp 258°.

Löwe, W. *et al*, *J. Het. Chem.*, 1995, **32**, 271 (*synth, pmr*)

2-Thiazolemethanol, 9CI, 8CI T-1-00111

2-(Hydroxymethyl)thiazole

[14542-12-2]



C_4H_5NOS M 115.1
$Bp_{0.2}$ 75-76°.

Hydrochloride: [23784-95-4]. Mp 126.5-127°.

Berlin, A.Y. *et al*, *Zh. Obshch. Khim.*, 1961, **31**, 1356; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1961, **31**, 1255 (*synth*)
Kazlauskas, R. *et al*, *Tet. Lett.*, 1977, 3183 (*pmr, cmr*)
Dondoni, A. *et al*, *Tetrahedron*, 1988, **44**, 2021 (*synth, pmr*)

4-Thiazolemethanol, 9CI, 8CI T-1-00112

4-(Hydroxymethyl)thiazole

[7036-04-6]

C_4H_5NOS M 115.1
Viscous oil. Bp_{15} 123-125°.

Picrate: Yellow needles (EtOH aq.). Mp 158-159°.

Ac:
$C_6H_7NO_2S$ M 157.1 Oil. Bp_{14} 117-119°, Bp_1 76°.

Mikhailov, B.M. *et al*, *Zh. Obshch. Khim.*, 1957, **27**, 726; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1957, **27**, 799 (*synth, Ac*)
Anderson, H.J. *et al*, *Can. J. Chem.*, 1964, **42**, 2375 (*Ac*)
U.S. Pat., 3 299 083, (1967); *CA*, **68**, 49592n (*synth*)

5-Thiazolemethanol, 9CI T-1-00113

5-(Hydroxymethyl)thiazole

[38585-74-9]

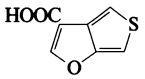
C_4H_5NOS M 115.1
Synthon for biologically active compds. Pale yellow oil. Mod. sol. H_2O. $Bp_{0.2}$ 76°.

Hydrochloride: Needles (EtOH). Mp 83-84°.
Picrate: Yellow needles (EtOH). Mp 152-154°.

Ac:
$C_6H_7NO_2S$ M 157.1 Oil. $Bp_{0.2}$ 70°.

Fallab, S., *Helv. Chim. Acta*, 1952, **35**, 215 (*synth, Ac*)
Kerdesky, F.A.J. *et al*, *Synth. Commun.*, 1995, **25**, 2639 (*synth, pmr*)

Thieno[3,4-*b*]furan-3-carboxylic acid T-1-00114

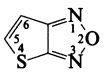


$C_7H_4O_3S$ M 168.1

Me ester:
$C_8H_6O_3S$ M 182.2 Prisms (petrol). Mp 63-64°.

Buttery, J.H. *et al*, *Aust. J. Chem.*, 1995, **48**, 593 (*synth, uv, pmr, cmr, ms*)

Thieno[2,3-*c*]furazan T-1-00115



$C_4H_2N_2OS$ M 126.1

1-Oxide: [52003-17-5]. *Thieno[3,2-c]furoxan*
$C_4H_2N_2O_2S$ M 142.1 Pale yellow needles (hexane). Mp 101-102° subl. Equilibrates in soln. to a mixt. of 1- and 3-oxides.

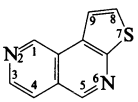
[57893-26-2]

Boulton, A.J. *et al*, *J.O.C.*, 1974, **39**, 2956 (*synth, pmr, ms*)
Paulmier, C. *et al*, *Bull. Soc. Chim. Fr.*, 1975, 1437 (*synth, pmr*)

Thieno[2,3-*c*][2,6]naphthyridine T-1-00116

Thieno[2,3-b][2,6]naphthyridine (*incorr.*)

[160351-10-0]



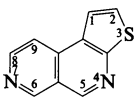
$C_{10}H_6N_2S$ M 186.2
Cryst. Mp 130-131°.

Björk, P. *et al*, *J. Het. Chem.*, 1994, **31**, 1161 (*synth, pmr, cmr*)

Thieno[2,3-*c*][2,7]naphthyridine T-1-00117

Thieno[2,3-b][2,7]naphthyridine (*incorr.*)

[160351-09-7]



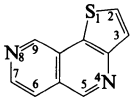
$C_{10}H_6N_2S$ M 186.2
Cryst. Mp 112-116°.

Björk, P. *et al*, *J. Het. Chem.*, 1994, **31**, 1161 (*synth, pmr, cmr*)

Thieno[3,2-*c*][2,6]naphthyridine T-1-00118

Thieno[3,2-b][2,6]naphthyridine (*incorr.*)

[160351-11-1]



$C_{10}H_6N_2S$ M 186.2

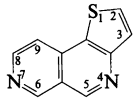
Cryst. Mp 131-132°.

Björk, P. *et al*, *J. Het. Chem.*, 1994, **31**, 1161 (*synth, pmr, cmr*)

Thieno[3,2-*c*][2,7] naphthyridine T-1-00119

*Thieno[3,2-*b*][2,7]naphthyridine (incorr.)*

[160351-19-9]



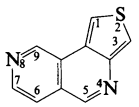
$C_{10}H_6N_2S$ M 186.2
Cryst. Mp 140-141°.

Björk, P. *et al*, *J. Het. Chem.*, 1994, **31**, 1161 (*synth, pmr, cmr*)

Thieno[3,4-*c*][2,6] naphthyridine T-1-00120

*Thieno[3,4-*b*][2,6]naphthyridine (incorr.)*

[160351-13-3]



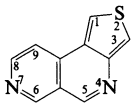
$C_{10}H_6N_2S$ M 186.2
Cryst. Mp 165-169°.

Björk, P. *et al*, *J. Het. Chem.*, 1994, **31**, 1161 (*synth, pmr, cmr*)

Thieno[3,4-*c*][2,7] naphthyridine T-1-00121

*Thieno[3,4-*b*][2,7]naphthyridine (incorr.)*

[160351-17-7]



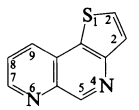
$C_{10}H_6N_2S$ M 186.2
Cryst. Mp 157-164°.

Björk, P. *et al*, *J. Het. Chem.*, 1994, **31**, 1161 (*synth, pmr, cmr*)

Thieno[2,3-*f*][1,7] naphthyridine T-1-00122

*Thieno[2,3-*b*][2,8]naphthyridine (incorr.)*

[160351-18-8]



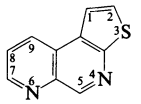
$C_{10}H_6N_2S$ M 186.2
Cryst. Mp 128-131°.

Björk, P. *et al*, *J. Het. Chem.*, 1994, **31**, 1161 (*synth, pmr, cmr*)

Thieno[3,2-*f*][1,7] naphthyridine T-1-00123

*Thieno[2,3-*b*][2,8]naphthyridine (incorr.)*

[56890-26-7]



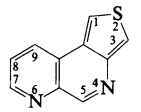
$C_{10}H_6N_2S$ M 186.2
Cryst. Mp 110-111°.

Björk, P. *et al*, *J. Het. Chem.*, 1994, **31**, 1161 (*synth, pmr, cmr*)

Thieno[3,4-*f*][1,7] naphthyridine T-1-00124

*Thieno[3,4-*b*][2,8]naphthyridine (incorr.)*

[160351-16-6]



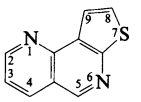
$C_{10}H_6N_2S$ M 186.2
Cryst. Mp 118-120°.

Björk, P. *et al*, *J. Het. Chem.*, 1994, **31**, 1161 (*synth, pmr, cmr*)

Thieno[2,3-*h*][1,6] naphthyridine T-1-00125

*Thieno[2,3-*b*][2,5]naphthyridine (incorr.)*

[141812-20-6]



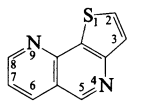
$C_{10}H_6N_2S$ M 186.2
Cryst. Mp 117-119°.

Malm, J. *et al*, *Tet. Lett.*, 1992, **33**, 2199 (*pmr, ms*)
Björk, P. *et al*, *J. Het. Chem.*, 1994, **31**, 1161 (*synth, cmr*)

Thieno[3,2-*h*][1,6] naphthyridine T-1-00126

*Thieno[2,3-*b*][2,5]naphthyridine (incorr.)*

[141812-18-2]



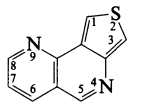
$C_{10}H_6N_2S$ M 186.2
Cryst. Mp 120-122°.

Malm, J. *et al*, *Tet. Lett.*, 1992, **33**, 2199 (*pmr, ms*)
Björk, P. *et al*, *J. Het. Chem.*, 1994, **31**, 1161 (*synth, cmr*)

Thieno[3,4-*h*][1,6]- naphthyridine T-1-00127

*Thieno[3,4-*b*][2,5]naphthyridine (incorr.)*

[141812-19-3]

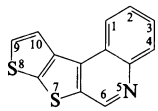


$C_{10}H_6N_2S$ M 186.2
Cryst. Mp 80-88°.

Malin, J. *et al*, *Tet. Lett.*, 1992, **33**, 2199 (*pmr, ms*)
Björk, P. *et al*, *J. Het. Chem.*, 1994, **31**, 1161 (*synth, cmr*)

Thieno[3′,2′:4,5]thieno[2,3-*c*] quinoline, 9CI T-1-00128

[120122-06-7]

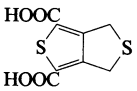


$C_{13}H_7NS_2$ M 241.3
Off-white cryst. (C_6H_6). Mp 203-204°.

Luo, J. *et al*, *J. Het. Chem.*, 1995, **32**, 317.

1*H*,3*H*-Thieno[3,4-*c*] thiophene-4,6-dicarboxylic acid, 9CI T-1-00129

[92223-90-0]



$C_8H_6O_4S_2$ M 230.2
Pink solid. Mp >350°.

Di-Me ester:
$C_{10}H_{10}O_4S_2$ M 258.3 Pink needles (THF/Et_2O). Mp 163-164°.

Diamide: [155632-46-5].
$C_8H_8N_2O_2S_2$ M 228.2 Pinkish microcryst. Mp >250°.

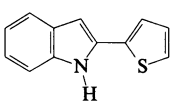
Dinitrile: [155632-45-4]. *4,6-Dicyano-1*H,*3*H-*thieno[3,4-*c*]thiophene*
$C_8H_4N_2S_2$ M 192.2 Needles (CH_2Cl_2/petrol). Mp 180-182°.

Wynberg, H. *et al*, *J.O.C.*, 1964, **29**, 1919 (*synth, Di-Me ester, pmr, uv*)
Beye, N. *et al*, *J.O.C.*, 1994, **59**, 2223 (*synth, deriv, pmr, cmr, ir, uv, ms*)

2-(2-Thienyl)-1*H*-indole, 9CI T-1-00130

2-(2-Indolyl)thiophene

[55968-16-6]



$C_{12}H_9NS$ M 199.2
Needles (C_6H_6/petrol). Mp 169° (162°).

Picrate: Long, dark red plates (petrol). Mp 137°.

Brunck, R., *Annalen*, 1893, **272**, 201 (*synth*)
Holla, B.S. *et al*, *J. Indian Chem. Soc.*, 1974, **51**, 965 (*synth*)

Holla, B.S. *et al, Indian J. Chem., Sect. B*, 1979, **17**, 187 (*ms*)
Tollari, S. *et al, J. Mol. Catal.*, 1994, **87**, 203 (*synth, pmr, ms*)

3-(2-Thienyl)-1*H*-indole, 9CI T-1-00131

2-(3-Indolyl)thiophene

[33333-57-2]

$C_{12}H_9NS$ M 199.2
Cryst. by subl. Mp 97-98°.

N-Me: [154010-91-0].
$C_{13}H_{11}NS$ M 213.3 No phys. props. reported.

Bergman, J., *Acta Chem. Scand.*, 1971, **25**, 1277 (*synth*)
Dekker, W.H. *et al, J. Agric. Food Chem.*, 1975, **23**, 785 (*synth*)
Couture, A. *et al, J.C.S. Perkin 1*, 1993, 2463 (*N-Me, synth, pmr*)

2-Thiocyanatothiophene T-1-00132

2-Thienyl thiocyanate, 9CI

[22552-32-5]

$C_5H_3NS_2$ M 141.2
Oil. Bp 220-230°, Bp_9 104°. n_D^{20} 1.5959.

▶ Lachrymator.

Cherbuliez, E. *et al, Helv. Chim. Acta*, 1952, **35**, 160 (*synth, uv*)
Söderbäck, E., *Acta Chem. Scand.*, 1954, **8**, 1851 (*synth*)
Gronowitz, S. *et al, Ark. Kemi*, 1960, **16**, 309 (*ir*)
Stoyanovich, F.M. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1969, 387; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1969, 337 (*synth*)
Toste, F.D. *et al, Synth. Commun.*, 1995, **25**, 1277 (*synth, ir, pmr, ms*)

3-Thiocyanatothiophene T-1-00133

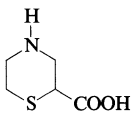
3-Thienyl thiocyanate, 9CI

[40507-55-9]

$C_5H_3NS_2$ M 141.2
Oil. Bp_{12} 114-115°. n_D^{20} 1.6035.

Gronowitz, S. *et al, Ark. Kemi*, 1960, **16**, 309 (*synth, ir*)
Gronowitz, S. *et al, J. Het. Chem.*, 1977, **14**, 281 (*synth*)

2-Thiomorpholinecarboxylic acid, 9CI T-1-00134



$C_5H_9NO_2S$ M 147.1

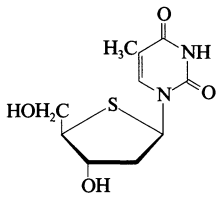
(±)-form

Hydrochloride: [88492-50-6].
Cryst. (EtOH/EtOAc). Mp 185-187°.
Nitrile: [107904-01-8]. *2-Cyanothiomorpholine*
$C_5H_8N_2S$ M 128.1 Liq. $Bp_{0.2}$ 88-90°.

Ricci, G. *et al, Biochim. Biophys. Acta*, 1983, **748**, 40 (*synth, ms*)
King, F.D. *et al, J. Med. Chem.*, 1993, **36**, 683 (*nitrile*)

4′-Thiothymidine, 9CI T-1-00135

[134111-33-4]



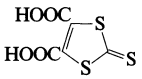
$C_{10}H_{14}N_2O_4S$ M 258.2
Cryst. (EtOH). Mp 213-215°.

Secrist, J.A. *et al, J. Med. Chem.*, 1991, **34**, 2361 (*synth, uv, pmr, cmr*)

2-Thioxo-1,3-dithiole-4,5-dicarboxylic acid, 9CI T-1-00136

Dimercaptomaleic acid cyclic trithiocarbonate, 8CI. 1,3-Dithiole-2-thione-4,5-dicarboxylic acid

[1008-62-4]



$C_5H_2O_4S_3$ M 222.2
Solid. Mp 165-167° (151-153°) dec.

Di-Me ester: [7396-41-0].
$C_7H_6O_4S_3$ M 250.3 Cryst. Mp 86-87° (72-72.5°).

Diamide: [1008-61-3].
$C_5H_4N_2O_2S_3$ M 220.2 Bright yellow solid. Mp 230° dec. approx.

Dinitrile: [1005-10-3]. *4,5-Dicyano-2-thioxo-1,3-dithiole*
$C_5N_2S_3$ M 184.2 Golden-yellow needles (methylcyclohexane). Mp 122-124°.

Dinitrile, 2-S-oxide: [1007-00-7].
$C_5N_2OS_3$ M 200.2 Purple cryst. (dioxan). Mp 190° dec.

▶ Intense skin irritant.

Klingsberg, E., *J.A.C.S.*, 1964, **86**, 5290 (*synth, dinitrile, diamide*)
O'Connor, B.R. *et al, J.O.C.*, 1970, **35**, 2002 (*Me ester synth*)
Melby, L.R. *et al, J.O.C.*, 1974, **39**, 2456 (*synth, Me ester, pmr*)

Thymotrinan, INN T-1-00137

Arginyllysylaspartic acid. Thymopoietin 32-34. RGH 0205. TP 3

[85465-82-3]

Arg-Lys-Asp

$C_{16}H_{31}N_7O_6$ M 417.4
Thymopoietin fragment.

L-L-L-form

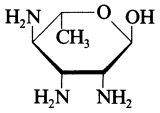
RGH 0205
Shows immunomodulatory, immunostimulant and antineoplastic activity. Phase II clinical trials (1991).

▶ CI9099033.

[85465-83-4]

Eur. Pat., 67 425, (1982) (*Gedeon Richter*); *CA*, **98**, 179924c (*synth*)
Kisfaludy, L. *et al, Hoppe Seyler's Z. Physiol. Chem.*, 1983, **364**, 933 (*synth, pharmacol*)
Iván, E. *et al, Arch. Toxicol., Suppl.*, 1985, **8**, 495 (*tox*)
Rajnavölgyi, E. *et al, Int. J. Immunopharmacol.*, 1986, **8**, 167 (*pharmacol*)
Szende, B. *et al, Immunopharmacol. Immunotoxicol.*, 1987, **9**, 19 (*pharmacol*)
Guo, W. *et al, J. Pharm. Biomed. Anal.*, 1993, **11**, 541 (*conformn*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 1421.

2,3,4-Triamino-2,3,4,6-tetradeoxymannose T-1-00138



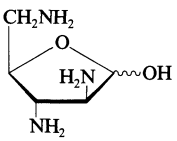
$C_6H_{15}N_3O_2$ M 161.2

α-L-Pyranose-form

Me glycoside, 2N,3N,4N-tri-Ac: [29788-90-7].
$C_{13}H_{23}N_3O_5$ M 301.3 Cryst. Mp 248-250°. $[\alpha]_D$ −98 (c, 0.5 in MeOH).

Lichtenthaler, F.W. *et al, Chem. Comm.*, 1970, 1081 (*Me gly deriv, pmr*)

2,3,5-Triamino-2,3,5-trideoxyarabinose T-1-00139



D-Furanose-*form*

$C_5H_{13}N_3O_2$ M 147.1

D-Furanose-form

2N,3N,5N-Tri-Ac: [53332-24-4].
$C_{11}H_{19}N_3O_5$ M 273.2 Amorph. powder. Mp 226-230° dec.

2N,3N,5N-Tribenzoyl: [55024-31-2].
$C_{26}H_{25}N_3O_5$ M 459.5 Cryst. ($CHCl_3$).

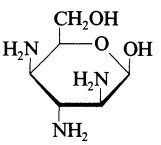
β-D-Furanose-form

Me glycoside: [53332-14-2].
$C_6H_{15}N_3O_2$ M 161.2 Needles ($MeOH/H_2O/Et_2O$) (as trihydrochloride). Mp 240° dec. (trihydrochloride). $[\alpha]_D^{19}$ −57.1 (c, 1.81 in H_2O). CAS no. refers to trihydrochloride.

Me glycoside, 2N,3N,5N-tri-Ac: [53332-21-1].
$C_{12}H_{21}N_3O_5$ M 287.3 Mp 293-294.5°. $[\alpha]_D$ −0.84 ($CHCl_3$/MeOH 4:1).

Kusumoto, S. *et al, Bull. Chem. Soc. Jpn.*, 1974, **4**, 2690 (D-fur deriv, β-D-fur deriv, ir)
Goto, T. *et al, Tet. Lett.*, 1974, 1413, 1417 (D-fur deriv, β-D-fur deriv)

2,3,4-Triamino-2,3,4-trideoxyidose T-1-00140



$C_6H_{15}N_3O_3$ M 177.2

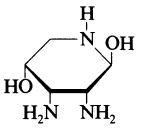
β-D-Pyranose-form

1,6-Anhydro: [15910-82-4].
$C_6H_{13}N_3O_2$ M 159.1 Cryst. + H_2O (dec.) (as trihydrochloride). Mp 189-190° (trihydrochloride). $[\alpha]_D^{20}$ −48.3 (c, 0.8 in H_2O). CAS no. refers to trihydrochloride.

*1,6-Anhydro, 2*N,*3*N,*4*N-*tri-Ac:* [15910-83-5].
$C_{12}H_{19}N_3O_5$ M 285.2 Needles (EtOH). Mp 267-268° (257-258°). $[\alpha]_D^{20}$ −50 (c, 1 in $CHCl_3$).

Lichtenthaler, F.W. *et al, Angew. Chem., Int. Ed.*, 1967, **6**, 568 (*tri-Ac, pmr*)
Lichtenthaler, F.W. *et al, Chem. Ber.*, 1968, **101**, 1846 (*anhydro, pmr*)

2,3,5-Triamino-2,3,5-trideoxyribose T-1-00141



β-D-Pyranose-*form*

$C_5H_{13}N_3O_2$ M 147.1

β-D-Pyranose-form

*2*N,*3*N,*5*N-*Tri-Ac:* [86204-40-2].
$C_{11}H_{19}N_3O_5$ M 273.2 Needles (EtOH). Mp 251°. $[\alpha]_D^{20}$ +36.5 (c, 0.5 in MeOH).

*1,2*N,*3*N,*4,5*N-*Penta-Ac:* [86204-42-4].
$C_{15}H_{23}N_3O_7$ M 357.3 Amorph. solid.

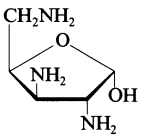
β-D-Furanose-form

*2*N,*3*N,*5*N-*Tri-Ac:* [86204-35-5].
$C_{11}H_{19}N_3O_5$ M 273.2 Prisms (EtOH/Et_2O). Mp 187-188°. $[\alpha]_D^{15}$ −10.5 (c, 0.3 in MeOH).

*Benzyl glycoside, 2*N,*3*N,*5*N-*tri-Ac:* [74593-12-7].
$C_{18}H_{25}N_3O_5$ M 363.4 Cryst. (EtOH/Et_2O). Mp 166°. $[\alpha]_D^{20}$ −74 (c, 0.3 in MeOH).

Hasegawa, A. *et al, Carbohydr. Res.*, 1980, **81**, 23 (*β-fur deriv, ir, pmr*)
Okumura, H. *et al, Agric. Biol. Chem.*, 1983, **47**, 839 (*β-fur deriv, β-pyr deriv, pmr*)

2,3,5-Triamino-2,3,5-trideoxyxylose T-1-00142



$C_5H_{13}N_3O_2$ M 147.1

α-D-Furanose-form

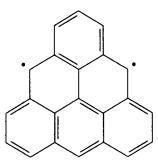
*1,2*N,*3*N,*5*N-*Tetra-Ac:* [74590-36-6].
$C_{13}H_{21}N_3O_6$ M 315.3 Needles (EtOH). Mp 229-231° dec. $[\alpha]_D^{20}$ +132 (c, 0.3 in DMF).

Hasegawa, A. *et al, Carbohydr. Res.*, 1980, **81**, 23 (*tetra-Ac, ir*)

Triangulene T-1-00143

Dibenzo[cd,mn]*pyrenediyl*

[126850-51-9]



$C_{22}H_{12}$ M 276.3

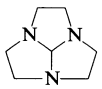
Non-Kekulé biradical. Currently known as a deriv. (see 4,8,12-Trioxodibenzo[*cd,mn*] pyrenediyl(3−), T-1-00255).

Allinson, G. *et al, J.C.S. Perkin 1*, 1995, 385.

1,4,7-Triazatricyclo[5.2.1.$0^{4,10}$] decane T-1-00144

*Hexahydro-6*bH-*2*a,*4*a,*6*a-*triazacyclopenta*[cd] *pentalene, 9CI.* [*9*]*Ane* N_3

[67705-38-8]



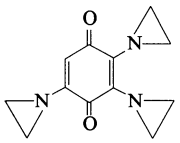
$C_7H_{13}N_3$ M 139.2
Oil. Mp −17° to −12° approx.

Atkins, T.J. *et al, J.A.C.S.*, 1980, **102**, 6365 (*synth, pmr*)
Weisman, G.R. *et al, Chem. Comm.*, 1987, 886 (*synth*)
Blake, A.J. *et al, Acta Cryst. C*, 1995, **41**, 738 (*cryst struct*)

Tri-1-aziridinyl-1,4-benzoquinone T-1-00145

2,3,5-Tris(1-aziridinyl)-2,5-cyclohexadiene-1,4-dione, 9CI. ***Triaziquone, BAN, INN.*** *Triaziquinone. Oncoredox. Trenimon. A 163. Bayer 3231. NSC 29215. Riker 601. RP 10257*

[68-76-8]



$C_{12}H_{13}N_3O_2$ M 231.2
Antineoplastic agent, can cross blood-brain barrier. No longer marketed. Purple cryst. (EtOAc). Mp 162.5-163°.

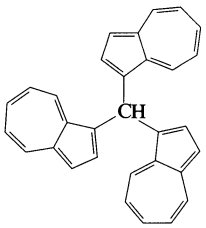
▶ LD_{50} (rat, ipr) 0.5 mg/kg. Exp. carcinogen and teratogen. DK7175000.

Gauss, W., *Chem. Ber.*, 1958, **91**, 2216 (*synth*)
U.S. Pat., 2 976 279, (1961) (*Schenley Industries*); *CA*, **55**, 18771h (*synth*)
Linford, J.H., *Chem. Biol. Interact.*, 1973, **6**, 149 (*rev, props*)
IARC Monog., 1975, **9**, 67; *Suppl.* 6, 545; *Suppl.* 7, 367 (*rev, tox*)
Obe, G. *et al, Mutat. Res.*, 1979, **65**, 21 (*rev*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, London, 1982/1989, 1873.
Silva, J.M. *et al, Cancer Res.*, 1992, **52**, 3015 (*tox*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, TND000.

Tri-1-azulenylmethane T-1-00146

1,1',1''-Methylidynetrisazulene

[115525-54-7]

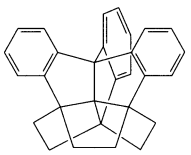


$C_{31}H_{22}$ M 394.5
Blue prisms. Mp 193-200° dec.

Ito, S. *et al, Bull. Chem. Soc. Jpn.*, 1995, **68**, 1409 (*synth, uv, pmr, cmr*)

Tribenzocentrohexaquinane T-1-00147

[157766-33-1]



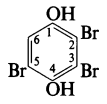
$C_{29}H_{24}$ M 372.5
Cryst. Mp 264°.

Kuck, D. *et al, Angew. Chem., Int. Ed.*, 1994, **33**, 1251 (*synth, pmr, cmr*)

2,3,5-Tribromo-1,4-benzenediol T-1-00148

Tribromohydroquinone. Tribromoquinol

[23149-36-2]



$C_6H_3Br_3O_2$ M 346.8
Constit. of a marine acorn worm. Needles ($CHCl_3$). Mp 136°.

Di-Ac: [23030-35-5].
$C_{10}H_7Br_3O_4$ M 430.8 Mp 186-190°.

Sarauw, E., *Annalen*, 1881, **209**, 116 (*synth*)
Terentev, A.P. *et al, Zh. Obshch. Khim.*, 1954, **24**, 1433; *CA*, **49**, 12353e (*synth*)
Higa, T. *et al, Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525 (*isol*)

3,4,4-Tribromo-3-buten-2-one T-1-00149

[70442-45-4]

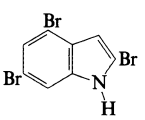
$Br_2C{=}CBrCOCH_3$

$C_4H_3Br_3O$ M 306.7
Constit. of the red seaweed *Asparagopsis taxiformis.*

Fenical, W. *et al, Proc. Int. Seaweed Symp.*, 1977, **9**, 387; *CA*, **91**, 14474.

2,4,6-Tribromo-1*H*-indole, 9CI T-1-00150

[128367-88-4]



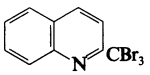
$C_8H_4Br_3N$ M 353.8
Alkaloid from the Okinawan red alga *Laurencia brongniartii*. Cryst. (hexane/CCl_4). Mp 106-113°.

Tanaka, J. *et al*, *Tetrahedron*, 1989, **45**, 7301 (*isol, ir, pmr, ms, struct*)

2-(Tribromomethyl)quinoline, 9CI T-1-00151

α,α,α-Tribromoquinaldine

[613-53-6]



$C_{10}H_6Br_3N$ M 379.8
Cryst. (EtOH or AcOH). Mp 130-132°.

Hammick, D.L., *J.C.S.*, 1923, 2883 (*synth*)
Hamana, M. *et al*, *Chem. Pharm. Bull.*, 1963, **11**, 411 (*synth*)

1,2,2-Tribromo-3,3,4,4,5,5,6,6,6-nonafluorohexane, 9CI T-1-00152

[59665-24-6]

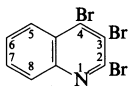
$F_3CCF_2CF_2CF_2CBr_2CH_2Br$

$C_6H_2Br_3F_9$ M 484.7
$Bp_{2.5}$ 97°.

Le Blanc, M. *et al*, *J. Fluorine Chem.*, 1976, **7**, 525.

2,3,4-Tribromoquinoline T-1-00153

[41320-97-2]



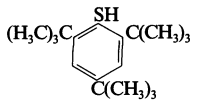
$C_9H_4Br_3N$ M 365.8
Cryst. (EtOH aq.). Mp 129-130°.

den Hertog, H.J. *et al*, *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1973, **92**, 304 (*synth, pmr*)

2,4,6-Tri-*tert*-butylbenzenethiol, 8CI T-1-00154

2,4,6-Tris(1,1-dimethylethyl)benzenethiol, 9CI

[961-39-7]



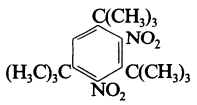
$C_{18}H_{30}S$ M 278.5
Cryst. (EtOH). Mp 180-181°.

Rundel, W., *Chem. Ber.*, 1968, **101**, 2956 (*synth*)

1,3,5-Tri-*tert*-butyl-2,4-dinitrobenzene T-1-00155

1,3,5-Tris(1,1-dimethylethyl)-2,4-dinitrobenzene, 9CI

[20568-98-3]



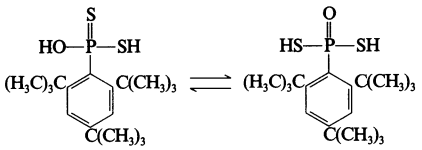
$C_{18}H_{28}N_2O_4$ M 336.4
Cryst. Mp 293-295°.

Myre, P.C. *et al*, *J.A.C.S.*, 1966, **88**, 1568; 1968, **90**, 2105; 1971, **93**, 3452 (*synth*)
Suzuki, H. *et al*, *J.C.S. Perkin 1*, 1993, 1591 (*synth, ir, pmr, ms*)

(2,4,6-Tri-*tert*-butylphenyl) phosphonodithioic acid, 8CI T-1-00156

[2,4,6-Tris(1,1-dimethylethyl)phenyl] phosphonodithioic acid, 9CI
Supermesitylphosphonodithioic acid

[97067-26-0]



$C_{18}H_{31}OPS_2$ M 358.5
Tautomeric.

Thiophosphoryl-form

O-*Me ester:* [89218-31-5]. O-*Methyl (2,4,6-tri*-tert-*butylphenyl)phosphonodithioate*
$C_{19}H_{33}OPS_2$ M 372.5 Cryst. (MeOH). Mp 70-71°.

O-*Et ester:* [122421-24-3]. O-*Ethyl (2,4,6-tri*-tert-*butylphenyl)phosphonodithioate*
$C_{20}H_{35}OPS_2$ M 386.6 Cryst. (MeOH). Mp 76-78°.

Navech, J. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1988, **39**, 33 (*synth, ir, pmr, cmr, P-31 nmr*)

1,2,3-Tri-*tert*-butyltriphosphine, 8CI T-1-00157

1,2,3-Tris(1,1-dimethylethyl)triphosphine, 9CI

[77256-93-0]

$(H_3C)_3CP[PHC(CH_3)_3]_2$

$C_{12}H_{29}P_3$ M 266.2
Ligand for Hf, Ti and Zr. Cryst. Diastereoisomers recognised spectroscopically.

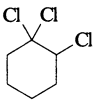
Di-Li salt: [91662-82-7].
Solid. Insol. pentane.

[69426-91-1]

Baudler, M. *et al*, *Z. Anorg. Allg. Chem.*, 1978, **446**, 169; 1984, **509**, 38, 53 (*synth, ir, Raman, pmr, P-31 nmr*)
Köpf, H. *et al*, *Chem. Ber.*, 1981, **114**, 2731 (*complexes*)
Baudler, M. *et al*, *Z. Anorg. Allg. Chem.*, 1992, **617**, 31 (*props*)

1,1,2-Trichlorocyclohexane, 9CI T-1-00158

[19024-48-7]



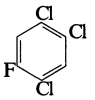
$C_6H_9Cl_3$ M 187.4

(±)-***form*** [29841-00-7]
Oil. Bp 222°, Bp_{20} 106-107°. n_D^{25} 1.5066.

Mousseron, M. *et al*, *Bull. Soc. Chim. Fr.*, 1953, 628 (*synth*)
Buys, H.R. *et al*, *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1967, **86**, 1007 (*conformn*)
Calderbank, K.E. *et al*, *J.C.S.(B)*, 1970, 1608 (*conformn*)
Brown, A.B. *et al*, *Synth. Commun.*, 1995, **25**, 485 (*synth, ir, pmr, cmr*)

1,2,4-Trichloro-5-fluorobenzene T-1-00159

[400-04-4]



$C_6H_2Cl_3F$ M 199.4
Needles (petrol). Mp 62-64°. Bp 203-204°.

Riemschneider, R., *Chem. Ber.*, 1958, **91**, 2605 (*synth*)
Vorozhtsov, N.N. *et al*, *Zh. Obshch. Khim.*, 1961, **31**, 1222; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1961, **31**, 1130.
Wasylishen, R. *et al*, *Can. J. Chem.*, 1970, **48**, 2885 (*pmr*)
Nyquist, R.A., *Spectrochim. Acta A*, 1970, **26**, 849 (*ir, Raman*)

P-(Trichloromethyl) phosphonous diamide, 9CI T-1-00160

$CCl_3P(NH_2)_2$

$CH_4Cl_3N_2P$ M 181.3

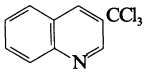
N,N,N′,N′-*Tetra-Me:* [100548-28-5].
N,N,N′,N′-*Tetramethyl*-P-(*trichloromethyl*) *phosphonous diamide.* (*Trichloromethyl*) *phosphonous bis(dimethylamide)*
$C_5H_{12}Cl_3N_2P$ M 237.4 Liq. Mp −1° to +1°. $Bp_{0.02}$ 62-64°. n_D^{20} 1.5021.

N,N,N′,N′-*Tetra-Et:* [110788-38-0].
N,N,N′,N′-*Tetraethyl*-P-(*trichloromethyl*) *phosphonous diamide.* (*Trichloromethyl*) *phosphonous bis(diethylamide)*
$C_9H_{20}Cl_3N_2P$ M 293.6 No phys. props. reported.

N,N,N′,N′-*Tetraisopropyl:* [123959-78-4].
N,N,N′,N′-*Tetraisopropyl*-P-(*trichloromethyl*)*phosphonous diamide.* (*Trichloromethyl*)*phosphonous bis(diisopropylamide)*
$C_{13}H_{28}Cl_3N_2P$ M 349.7 Cryst. (pentane). Mp 99-100°.

Prishchenko, A.A. *et al*, *Zh. Obshch. Khim.*, 1985, **55**, 1194; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1985, **55**, 1065 (*tetramethyl, synth, pmr, cmr, P-31 nmr*)
Marchenko, A.P. *et al*, *Zh. Obshch. Khim.*, 1986, **56**, 1910; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1986, **56**, 1687 (*tetraethyl, synth, P-31 nmr*)
Koidan, G.N. *et al*, *Zh. Obshch. Khim.*, 1988, **58**, 1461; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1988, **58**, 1304 (*tetramethyl, synth, P-31 nmr*)
Marchenko, A.P. *et al*, *Zh. Obshch. Khim.*, 1989, **59**, 959; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1989, **59**, 843 (*tetraisopropyl, synth, cmr, P-31 nmr*)

3-(Trichloromethyl)quinoline T-1-00161

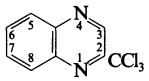


$C_{10}H_6Cl_3N$ M 246.5

Oil. $Bp_{0.2}$ 83-85°.

Cartwright, D. *et al, J.C.S. Perkin 1*, 1995, 2595 (*synth, pmr*)

2-(Trichloromethyl) quinoxaline T-1-00162



$C_9H_5Cl_3N_2$ M 247.5
Cryst. Mp 57°. $Bp_{0.5}$ 120°.

Cartwright, D. *et al, J.C.S. Perkin 1*, 1995, 2595 (*synth, pmr*)

3,3,3-Trichloro-1-phenylpropene T-1-00163

(3,3,3-Trichloro-1-propenyl)benzene, 9CI. ω-Trichloromethylstyrene

$PhCH{=}CHCCl_3$

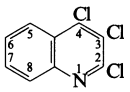
$C_9H_7Cl_3$ M 221.5
Oil. Bp_1 91-92°.

[76707-82-9, 91083-81-7]

Kharasch, M.S. *et al, J.A.C.S.*, 1947, **69**, 1105 (*synth*)
Nesmeyanov, A.N. *et al, Zh. Obshch. Khim.*, 1956, **25**, 1070; *J. Gen. Chem. USSR (Engl. Transl.)*, 1956, **25**, 1215 (*synth*)
Voges, A. *et al, Synthesis*, 1995, 253 (*synth, pmr, cmr*)

2,3,4-Trichloroquinoline T-1-00164

[40335-02-2]



$C_9H_4Cl_3N$ M 232.4
Needles (MeOH). Mp 106-107°.

Beak, P. *et al, Tetrahedron*, 1972, **28**, 5507 (*synth, pmr, ir, ms*)
Osborne, A.G. *et al, J.C.S. Perkin 1*, 1993, 2747 (*synth, pmr, cmr*)

1,14-Tricosadiene T-1-00165

$H_3C(CH_2)_7CH{=}CH(CH_2)_{11}CH{=}CH_2$

$C_{23}H_{44}$ M 320.6

(E)-form [104899-43-6]
Isol. from the green alga *Botryococcus braunii.*

(Z)-form [104899-38-9]
Isol. from *B. braunii.*

Metzger, P. *et al, Phytochemistry*, 1986, **25**, 1869; 1993, **33**, 1125 (*isol, pmr, cmr*)

Tricosafluorododecanoic acid, 9CI T-1-00166

[307-55-1]

$F_3C(CF_2)_{10}COOH$

$C_{12}HF_{23}O_2$ M 614.1
Cryst. (CCl_4). Mp 112-114°.

Hare, E.F. *et al, J. Phys. Chem.*, 1954, **58**, 236 (*props*)
Huang, B.-N., *J. Fluorine Chem.*, 1987, **36**, 49 (*synth, ir, F-19 nmr*)

10-Tricosanone T-1-00167

[39754-76-2]

$H_3C(CH_2)_{12}CO(CH_2)_8CH_3$

$C_{23}H_{46}O$ M 338.6
Constit. of the seeds of *Achyranthes aspera.* Mp 60-61°.

Larson, G.L. *et al, J.O.C.*, 1985, **50**, 5260 (*synth*)
Ali, M., *Orient. J. Chem.*, 1993, **9**, 84 (*isol*)

1-Tricosene T-1-00168

[18835-32-0]

$H_3C(CH_2)_{20}CH{=}CH_2$

$C_{23}H_{46}$ M 322.6
Constit. of the alga *Botryococcus braunii* and various plant spp. incl. *Gardenia tahitensis.* Fp 41.6°. Bp 379°, Bp_{10} 222.4°.

Dreisbach, R.R., *Adv. Chem. Ser.*, 1959, **22**, 1 (*props*)
Bessiere, J.M. *et al, Fitoterapia*, 1985, **56**, 62 (*isol*)
MacLeod, G., *Phytochemistry*, 1990, **29**, 1197 (*isol*)
Davis, F. *et al, Macromolecules*, 1991, **56**, 5695 (*synth*)
Metzger, P., *Phytochemistry*, 1993, **33**, 1125 (*isol*)

(Tricyanomethyl)phosphonic acid T-1-00169

Tricyanomethanephosphonic acid

$(NC)_3CP(O)(OH)_2$

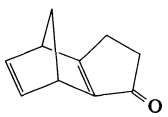
$C_4H_2N_3O_3P$ M 171.0

Bis(2-methylpropyl) ester: [111670-81-6].
$C_{12}H_{18}N_3O_3P$ M 283.2 Viscous oil.

Di-Ph ester:
$C_{16}H_{10}N_3O_3P$ M 323.2 Viscous oil.

Koehler, H. *et al, Z. Anorg. Allg. Chem.*, 1986, **542**, 53 (*synth, ir, P-31 nmr*)

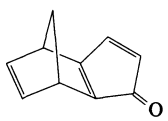
Tricyclo[5.2.1.$0^{2,6}$]deca-2(6),8-dien-3-one T-1-00170



$C_{10}H_{10}O$ M 146.1
Oil.

Zhu, J. *et al, Tetrahedron*, 1995, **51**, 5117 (*synth, ir, pmr, cmr, ms*)

Tricyclo[5.2.1.$0^{2,6}$]deca-2(6),4,8-trien-3-one T-1-00171

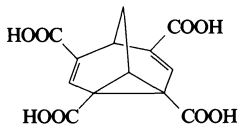


$C_{10}H_8O$ M 144.1
Reactive intermed., can be trapped by cycloaddn. or nucleophilic conjugate addn.

Zhu, J. *et al, Tetrahedron*, 1995, **51**, 5117 (*synth*)

Tricyclo[3.3.1.$0^{2,8}$]nona-3,6-diene-2,4,6,8-tetracarboxylic acid, 9CI T-1-00172

2,4,6,8-Barbaralanetetracarboxylic acid



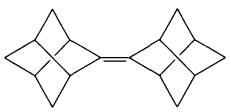
$C_{13}H_{10}O_8$ M 294.2

Tetra-Me ester: [155671-79-7].
$C_{17}H_{18}O_8$ M 350.3 Cryst. (Et_2O/hexane). Mp 99-100°.

Win, W.W. *et al, J.O.C.*, 1994, **59**, 2803 (*synth, cryst struct, ir, pmr, uv*)

2-Tricyclo[3.3.0.$0^{3,7}$] octylidenetricyclo[3.3.0.$0^{3,7}$] octane, 9CI T-1-00173

2,2′-Bi(tricyclo[3.3.0.$0^{3,7}$]oct-2-ylidene)



$C_{16}H_{20}$ M 212.3
Two isomers obt., the C_{2h}-symmetric (±)-form (illus.) and the D_2-symmetric *meso*-form.

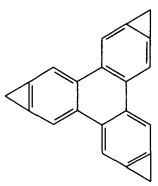
(±)-form
Needles. Mp 30°.

meso-form
Needles. Mp 30°.

[169275-26-7]

Gleiter, R. *et al, Angew. Chem., Int. Ed.*, 1995, **34**, 1001.

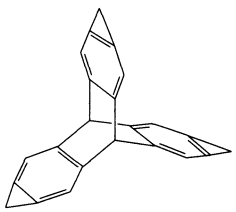
2,3:6,7:10,11-Tricyclopropatriphenylene T-1-00174



$C_{21}H_{12}$ M 264.3
Solid.

Billups, W.E. *et al, J.A.C.S.*, 1994, **116**, 8831 (*synth, uv, pmr, cmr*)

2,3:6,7:14,15-Tricyclopropatriptycene T-1-00175



$C_{23}H_{14}$ M 290.3
Solid.

Billups, W.E. *et al, J.A.C.S.*, 1994, **116**, 8831 (*synth, ir, uv, pmr*)

1,12-Tridecadiene, 9CI T-1-00176

[21964-48-7]

$H_2C{=}CH(CH_2)_9CH{=}CH_2$

$C_{13}H_{24}$ M 180.3
Liq. Bp_{56} 139-140°, Bp_{17} 111.4-111.8°. n_D^{25} 1.4400.

Marvel, C.S. *et al*, *J.A.C.S.*, 1959, **81**, 4737 (*synth*)
Johnson, D.K. *et al*, *Synth. Commun.*, 1994, **24**, 1557 (*synth, pmr*)

5,11-Tridecadiyn-1-ol T-1-00177

[160109-69-3]

$H_3CC{\equiv}C(CH_2)_4C{\equiv}C(CH_2)_3CH_2OH$

$C_{13}H_{20}O$ M 192.3
No phys. props. descr.

Bao, J. *et al*, *J.A.C.S.*, 1994, **116**, 7616 (*synth, ir, pmr, cmr, ms*)

Tridecafluoroheptanoic acid T-1-00178

Perfluoroheptanoic acid

[375-85-9]

$F_3C(CF_2)_5COOH$

$C_7HF_{13}O_2$ M 364.0
Cryst. (CCl_4). d 1.79. Mp 54°. Bp 175°, Bp_{40} 105°.

Na salt: [20109-59-5].
Cryst. (H_2O).

Me ester: [14312-89-1].
$C_8H_3F_{13}O_2$ M 378.0 Liq. Bp_3 60.65°.

Amide: [2358-22-7].
$C_7H_2F_{13}NO$ M 363.0 Cryst. (MeOH aq.). Mp 135°.

Nitrile: [62038-08-8].
Tridecafluoroheptanenitrile. Perfluoroheptanenitrile. 1-Cyanotridecafluorohexane
$C_7F_{13}N$ M 345.0 Bp 80°.

[21049-36-5, 52447-22-0]

Battais, A. *et al*, *J. Fluorine Chem.*, 1981, **19**, 35 (*synth*)
Thoai, N. *et al*, *J. Fluorine Chem.*, 1982, **20**, 271 (*nitrile*)
Afzal, J. *et al*, *J. Fluorine Chem.*, 1986, **34**, 385 (*synth, derivs*)
Wrackmeyer, B. *et al*, *J. Fluorine Chem.*, 1987, **35**, 359 (*cmr, O-17 nmr*)
Huang, B.-N. *et al*, *J. Fluorine Chem.*, 1987, **36**, 49 (*synth, ir, F-19 nmr*)
Benefice-Malouet, S. *et al*, *Synthesis*, 1991, 647 (*synth, bibl*)

1,1,2,2,3,3,4,4,5,5,6,6,6-Tridecafluoro-1-hexanesulfenyl chloride, 9CI T-1-00179

Perfluorohexanesulfenylchloride

[89987-98-4]

$F_3C(CF_2)_5SCl$

$C_6ClF_{13}S$ M 386.5
Catalyst in redn. of OH groups. Bp 124-126°.

Cole, S.J. *et al*, *J.C.S. Perkin 1*, 1991, 103 (*use*)

(Triethoxymethyl)phosphonic acid T-1-00180

$(EtO)_3CP(O)(OH)_2$

$C_7H_{17}O_6P$ M 228.1

Di-Et ester: [17507-52-7]. *Diethyl [(triethoxy)methyl]phosphonate*
$C_{11}H_{25}O_6P$ M 284.2 Liq. Bp_1 85°. n_D^{20} 1.4252.

Diisopropyl ester: [17391-59-2]. *Diisopropyl [(triethoxy)methyl]phosphonate*
$C_{13}H_{29}O_6P$ M 312.3 Liq. Bp_1 83°. n_D^{20} 1.4220.

Dibutyl ester: [17507-53-8]. *Dibutyl [(triethoxy)methyl]phosphonate*
$C_{15}H_{33}O_6P$ M 340.3 Liq. Bp_1 111°. n_D^{20} 1.4295.

Prishchenko, A.A. *et al*, *Zh. Obshch. Khim.*, 1988, **58**, 2168; *J. Gen. Chem. USSR (Engl. Transl.)*, 1988, **58**, 1932 (*synth, cmr, P-31 nmr*)

1,1,1-Trifluoro-4-bromobutane T-1-00181

[406-81-5]

$F_3CCH_2CH_2CH_2Br$

$C_4H_6BrF_3$ M 190.9
d_{25} 1.58. Bp 103-105°. n_D^{25} 1.3800.

Gavlin, G. *et al*, *J.O.C.*, 1956, **21**, 1342 (*synth*)
Steward, O.W. *et al*, *J.A.C.S.*, 1959, **81**, 1983 (*synth*)

4,4,4-Trifluoro-1-butanol T-1-00182

[461-18-7]

$F_3CCH_2CH_2CH_2OH$

$C_4H_7F_3O$ M 128.0
Bp 123-125°. n_D^{20} 1.3516 (1.3410).

4-Nitrobenzoyl: Mp 47.5-48°.
3,5-Dinitrobenzoyl: Mp 86.5-97°.

McBee, E.T., *J.A.C.S.*, 1950, **72**, 5071 (*synth*)
Walborsky, H.M. *et al*, *J.A.C.S.*, 1955, **77**, 3637 (*synth*)
Gavlin, G. *et al*, *J.O.C.*, 1956, **21**, 1342 (*synth*)

4,4,4-Trifluoro-2-butanone T-1-00183

[2366-70-3]

$F_3CCH_2COCH_3$

$C_4H_5F_3O$ M 126.0
Bp 95-96°.

2,4-Dinitrophenylhydrazone: Mp 131-132°.

Haszeldine, R.N. *et al*, *J.C.S.*, 1954, 1261 (*synth, ir*)
Tordeux, M. *et al*, *Org. Magn. Reson.*, 1980, **14**, 407 (*nmr*)
Muller, N., *J.O.C.*, 1983, **48**, 1370 (***synth***)

P-(Trifluoroethenyl) phosphonous diamide, 9CI T-1-00184

P-(*Trifluorovinyl*)*phosphonous diamide*

$F_2C{=}CFP(NH_2)_2$

$C_2H_4F_3N_2P$ M 144.0

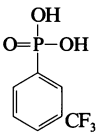
N,N,N′,N′-*Tetra-Me:* [24512-26-3].
N,N,N′,N′-*Tetramethyl*-P-(*trifluoroethenyl*) *phosphonous diamide. (Trifluorovinyl) phosphonous bis(dimethylamide)*
$C_6H_{12}F_3N_2P$ M 200.1 Condensed at −78°. Dec. within hrs. at r.t.

N,N,N′,N′-*Tetra-Et:* N,N,N′,N′-*Tetraethyl*-P-(*trifluoroethenyl*)*phosphonous diamide. (Trifluorovinyl)phosphonous bis(diethylamide)*
$C_{10}H_{20}F_3N_2P$ M 256.2 Unpleasant smelling liq. d_4^{20} 1.05. Bp_{11} 89-90°. n_D^{20} 1.4470.

Sterlin, R.N. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1960, 1991; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1960, 1851 (*tetraethyl*)
Cowley, A.H. *et al*, *J.A.C.S.*, 1969, **91**, 1929 (*tetramethyl, synth, pmr, F-19 nmr*)

[3-(Trifluoroethyl)phenyl] phosphonic acid, 9CI T-1-00185

[51907-90-5]



$C_7H_6F_3O_3P$ M 226.0
Solid or plates (H_2O). Mp 116° (112-113°).

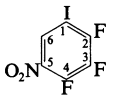
Di-Me ester: [42250-24-8]. *Dimethyl [3-(trifluoromethyl)phenyl]phosphonate*
$C_9H_{10}F_3O_3P$ M 254.1 Liq. $Bp_{1.25}$ 88-90°.

Di-Et ester: [54057-97-5]. *Diethyl [3-(trifluoromethyl)phenyl]phosphonate*
$C_{11}H_{14}F_3O_3P$ M 282.1 Phys. props. not reported.

Bentrude, W.G. *et al*, *J.A.C.S.*, 1972, **95**, 3625 (*dimethyl ester, synth, ir, pmr*)
Schmutzler, R., *J.C.S. Dalton*, 1973, 2687 (*synth, F-19 nmr, P-31 nmr*)
Bunnett, J.F. *et al*, *J.O.C.*, 1974, **39**, 3612 (*diethyl ester*)
Klumpp, E. *et al*, *Chem. Ber.*, 1989, **122**, 2021 (*synth*)

2,3,4-Trifluoro-1-iodo-5-nitrobenzene T-1-00186

[148388-75-4]



$C_6HF_3INO_2$ M 302.9
Liq. $Bp_{0.1}$ 55-57°.

Olah, G.A. *et al*, *J.O.C.*, 1993, **58**, 3194 (*synth, cmr, ms*)

1,1,1-Trifluoro-3-iodopropane T-1-00187

[460-37-7]

$F_3CCH_2CH_2I$

$C_3H_4F_3I$ M 223.9
Bp 90°. n_D^{25} 1.4175.

Haszeldine, R.N., *J.C.S.*, 1949, 2856; 1953, 1764 (*synth, uv*)
Bell, T.N., *J.C.S.*, 1961, 4973.

3′-(Trifluoromethyl) acetophenone, 8CI T-1-00188

1-[3-(Trifluoromethyl)phenyl]ethanone, 9CI. m-*Acetylbenzotrifluoride*

[349-76-8]

$C_9H_7F_3O$ M 188.1
d 1.23. Bp 198-200°.

Semicarbazone: [454-05-7].
Mp 201-203°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1243A.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 25C.
Eistert, B. *et al*, *Annalen*, 1968, **717**, 80 (*synth, ir*)

4′-(Trifluoromethyl) acetophenone T-1-00189

1-[4-(Trifluoromethyl)phenyl]ethanone, 9CI. p-*Acetylbenzotrifluoride*

[709-63-7]

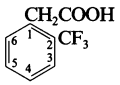
$C_9H_7F_3O$ M 188.1
Mp 30-33°. Bp_8 79-80°.

Hortmann, A.G. *et al*, *J.O.C.*, 1972, **37**, 322 (*synth, bibl, pmr*)

2-(Trifluoromethyl) benzeneacetic acid T-1-00190

(α,α,α-*Trifluoro-o-tolyl*)*acetic acid*

[3038-48-0]



$C_9H_7F_3O_2$ M 204.1
Mp 104-106°.

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 150B.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 146C.
Van der Stelt, C. *et al*, *Arzneim.-Forsch.*, 1965, **15**, 1251 (*synth*)

3-(Trifluoromethyl) benzeneacetic acid T-1-00191

(α,α,α-*Trifluoro-m-tolyl*)*acetic acid*

[351-35-9]

$C_9H_7F_3O_2$ M 204.1
Cryst. (petrol). Mp 76-79°.

Me ester: [62451-84-7].
$C_{10}H_9F_3O_2$ M 218.1 $Bp_{0.2}$ 57-58°.

Et ester:
$C_{11}H_{11}F_3O_2$ M 232.2 Bp_4 87-88°.

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 154C.
Corse, J.W. *et al*, *J.A.C.S.*, 1948, **70**, 2837 (*synth*)
Rosenkrantz, B.E. *et al*, *J. Chem. Eng. Data*, 1963, **8**, 237 (*synth, Et ester*)
Lambert, J.B. *et al*, *J.A.C.S.*, 1977, **99**, 3059 (*synth, Me ester*)

4-(Trifluoromethyl) benzeneacetic acid T-1-00192

(α,α,α-*Trifluoro-p-tolyl*)*acetic acid.* (*4-Trifluoromethylphenyl*)*acetic acid*

[32857-62-8]

$C_9H_7F_3O_2$ M 204.1
Mp 83-85°.

Et ester: [721-63-1].
$C_{11}H_{11}F_3O_2$ M 232.2 Mp 34-35°, Mp 130-135°. Bp_7 104-105°. No explanation for wide literature discrepancy in Mp's.

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 157A.
Rosenkrantz, B.E. *et al*, *J. Chem. Eng. Data*, 1963, **8**, 237 (*synth, Et ester*)
U.K. Pat., 1 310 642, (1973); *CA*, **79**, 5358p (*synth*)
Hammond, G.B. *et al*, *J. Fluorine Chem.*, 1988, **40**, 81 (*synth, Et ester, ir, pmr*)

2-(Trifluoromethyl) benzophenone, 8CI T-1-00193

Phenyl[*2-(trifluoromethyl)phenyl*]*methanone, 9CI*

[727-99-1]

$C_{14}H_9F_3O$ M 250.2
Cryst. Mp 60-62°. Bp_{31} 175-178°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1271D.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 66D.
Lichtenberger, J. *et al*, *Bull. Soc. Chim. Fr.*, 1962, 587 (*synth*)
Van der Stelt, C. *et al*, *Arzneim.-Forsch.*, 1964, **14**, 864 (*synth*)

3-(Trifluoromethyl) benzophenone T-1-00194

Phenyl[*3-(trifluoromethyl)phenyl*]*methanone, 9CI*

[728-81-4]

$C_{14}H_9F_3O$ M 250.2
Mp 52-53°. $Bp_{1.5}$ 121-123°.

Oxime: [732-47-8].
Mp 134-141°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1272A.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 67A.
Kovacic, P. *et al*, *J.O.C.*, 1961, **26**, 2541 (*synth*)
Lichtenberger, J. *et al*, *Bull. Soc. Chim. Fr.*, 1962, 587 (*synth*)
Hoffman, R.V. *et al*, *J.O.C.*, 1979, **44**, 2364 (*synth*)

4-(Trifluoromethyl) benzophenone, 8CI T-1-00195

Phenyl[*4-(trifluoromethyl)phenyl*]*methanone, 9CI*

[728-86-9]

$C_{14}H_9F_3O$ M 250.2
Cryst. Mp 116-118°.

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 63D.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 67B.
Rooney, C.S. *et al*, *Can. J. Chem.*, 1955, **33**, 1633 (*synth*)
Hugel, H.M. *et al*, *Aust. J. Chem.*, 1979, **32**, 1511 (*cmr*)

2-(Trifluoromethyl)benzyl alcohol, 8CI T-1-00196

2-(Trifluoromethyl)benzenemethanol, 9CI

[346-06-5]

$C_8H_7F_3O$ M 176.1
d 1.33. Bp_{20} 90°.

3,5-Dinitrobenzoyl: Mp 73-74°.

Aldrich Library of FT-IR Spectra, 1st edn., **3**, 1051C.
Aldrich Library of NMR Spectra, 2nd edn., **1**, 932A.
Filler, R. *et al*, *J.O.C.*, 1960, **25**, 733 (*synth, deriv*)

3-(Trifluoromethyl)benzyl alcohol T-1-00197

3-(Trifluoromethyl)benzenemethanol, 9CI

[349-75-7]

$C_8H_7F_3O$ M 176.1
Liq. d 1.29. Bp_2 68°.

Szmant, H.H., *J.A.C.S.*, 1950, **72**, 1419 (*synth*)
Blanco, F.E. *et al*, *J.O.C.*, 1977, **42**, 868 (*synth, ir, pmr*)

4-(Trifluoromethyl)benzyl alcohol T-1-00198

4-(Trifluoromethyl)benzenemethanol, 9CI

[349-95-1]

$C_8H_7F_3O$ M 176.1
d 1.29. Bp_4 78-80°.

Hass, H.B. *et al*, *J.A.C.S.*, 1949, **71**, 1767 (*synth*)
Smith, P.J. *et al*, *Can. J. Chem.*, 1970, **48**, 125 (*synth*)
Miller, D.J. *et al*, *J.O.C.*, 1981, **46**, 4247 (*synth, bibl*)

2-(Trifluoromethyl) benzylamine T-1-00199

2-(Trifluoromethyl)benzenemethanamine, 9CI

[3048-01-9]

$C_8H_8F_3N$ M 175.1
Inhibits phenethanolamine *N*-methyl transferase and aids clot lysis. d 1.25. Bp_{64} 108-110°. n_D^{25} 1.4673.

Hydrochloride: [2944-97-0].
Mp 286-288°.

Freifelder, M. *et al*, *J. Pharm. Sci.*, 1965, **54**, 1204 (*synth*)

3-(Trifluoromethyl) benzylamine, 8CI T-1-00200

3-(Trifluoromethyl)benzenemethanamine, 9CI

[2740-83-2]

$C_8H_8F_3N$ M 175.1

Inhibits phenethanolamine *N*-methyl transferase and aids clot lysis. d 1.22. Bp_{28} 93-97°. n_D^{25} 1.4613.

Hydrochloride: [2944-96-9].
Cryst. (MeOH/Et_2O). Mp 178-180°.

Freifelder, M. *et al, J. Pharm. Sci.*, 1965, **54**, 1204 (*synth*)
Meindl, W.R. *et al, J. Med. Chem.*, 1984, **27**, 1111 (*synth*)

4-(Trifluoromethyl) benzylamine, 8CI T-1-00201

4-(Trifluoromethyl)benzenemethanamine, 9CI

[3300-51-4]

$C_8H_8F_3N$ M 175.1

Inhibits phenethanolamine *N*-Me transferase and aids clot lysis. d 1.23. Bp_{51} 114-120°, Bp_{15} 80-82°. n_D^{25} 1.4630.

Hydrochloride: [3047-99-2].
Cryst. (MeOH/Et_2O). Mp 194-198°, Mp 276°.

Freifelder, M. *et al, J. Pharm. Sci.*, 1965, **54**, 1204 (*synth*)
Meindl, W.R. *et al, J. Med. Chem.*, 1984, **27**, 1111 (*synth*)

1,1,1-Trifluoro-3-methylbutane T-1-00202

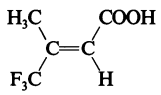
[406-49-5]

$(H_3C)_2CHCH_2CF_3$

$C_5H_9F_3$ M 126.1
d_{25} 0.98. Bp 31°. n_D^{25} 1.3226.

Tarrant, P. *et al, J.A.C.S.*, 1954, **76**, 2343 (*synth*)

4,4,4-Trifluoro-3-methyl-2-butenoic acid, 9CI T-1-00203



$C_5H_5F_3O_2$ M 154.0

(*E*)-*form* [400-28-2]
β-Trifluoromethylcrotonic acid
Low melting cryst. Mp 29.5-31°. Bp 182°, Bp_{21} 80-81°.

Me ester:
$C_6H_7F_3O_2$ M 168.1 Liq. d_4^{20} 1.21. Bp_{753} 112.5-113.5°. n_D^{20} 1.3718.

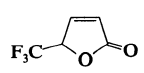
[93404-33-2]

Walborsky, H.M. *et al, J.A.C.S.*, 1955, **77**, 3637 (*synth*)
Knunyants, I.L. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1961, 1057; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1961, 977 (*synth*)
Nemoto, H. *et al, J.O.C.*, 1995, **60**, 594 (*synth, ir, pmr*)

5-(Trifluoromethyl)-2(5*H*)-furanone, 9CI T-1-00204

4-Trifluoromethyl-2-buten-4-olide

[2253-15-8]



$C_5H_3F_3O_2$ M 152.0

(±)-*form*
d_4^{20} 1.44. Bp_{12-13} 83°, Bp_{30} 100-105°. n_D^{20} 1.3853.

3,4-Dihydro:
$C_5H_5F_3O_2$ M 154.0 Liq. d_4^{20} 1.413. Bp_{25} 78-79°. n_D^{20} 1.3748.

Groth, R.H., *J.O.C.*, 1959, **24**, 1709 (*synth, props*)
Filler, R. *et al, Can. J. Chem.*, 1967, **45**, 1018 (*synth*)
Yoshida, M. *et al, J.C.S. Perkin 1*, 1993, 501 (*synth, pmr, cmr, ir*)

2-(Trifluoromethyl)-1,1,1,3,3,3-hexafluoropropane, 8CI T-1-00205

Tris(trifluoromethyl)methane

[382-24-1]

$(F_3C)_3CH$

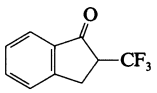
C_4HF_9 M 220.0
Bp 12-14°.

Knunyants, I.L. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1960, 1693 (*synth*)
Andreades, S., *J.A.C.S.*, 1964, **86**, 2003 (*synth, ms, ir, F-19 nmr*)
Knunyants, I.L. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1965, **165**, 827 (*synth*)

2-(Trifluoromethyl)-1-indanone T-1-00206

2,3-Dihydro-2-(trifluoromethyl)-1H-inden-1-one, 9CI

[157364-39-1]



$C_{10}H_7F_3O$ M 200.1

(±)-*form*
Cryst. (hexane). Mp 67.3-67.9°.

Umemoto, T. *et al, J.O.C.*, 1994, **59**, 5692 (*synth, pmr, ir, F-19 nmr*)

(3-Trifluoromethylphenyl) phosphonous dichloride T-1-00207

[51907-89-2]

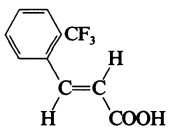
$C_7H_4Cl_2F_3P$ M 246.9
Liq. $Bp_{0.07}$ 42°. n_D^{26} 1.5214.

Schmutzler, R., *J.C.S. Dalton*, 1973, 2687 (*synth, F-19 nmr, P-31 nmr*)
Kruczynski, L.J. *et al, Can. J. Chem.*, 1990, **68**, 488 (*synth, props*)

3-[2-(Trifluoromethyl)phenyl]-2-propenoic acid, 9CI T-1-00208

2-(Trifluoromethyl)cinnamic acid, 8CI

[2062-25-1]



$C_{10}H_7F_3O_2$ M 216.1

(*E*)-*form* [98386-81-3]
Cryst. Mp 205-207°.

Me ester: [157518-53-1].
$C_{11}H_9F_3O_2$ M 230.1 Oil. $Bp_{0.01}$ 66-68°.

[50620-98-9, 74738-22-0]

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 175D.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 172C.
Filler, R. *et al, J. Chem. Eng. Data*, 1964, **9**, 370 (*synth, uv*)
Vallgarda, J. *et al, J.C.S. Perkin 1*, 1994, 461 (*synth, pmr, cmr, Me ester*)

3-[3-(Trifluoromethyl)phenyl]-2-propenoic acid, 9CI T-1-00209

3-(Trifluoromethyl)cinnamic acid, 8CI

[779-89-5]

$C_{10}H_7F_3O_2$ M 216.1

(*E*)-*form* [67801-07-4]
Needles. Mp 135.5-136.5°.

Chloride: [64379-91-5].
$C_{10}H_6ClF_3O$ M 234.6 d 1.37. Bp_{60} 148°. n_D^{20} 1.5440.

Nitrile: [58177-64-3].
$C_{10}H_6F_3N$ M 197.1 Bp_{27} 140-142°.

(*Z*)-*form* [16642-87-8]
Cryst. Mp 53.5-54.5°.

[58177-61-0, 60689-14-7, 64380-24-1, 87087-35-2, 93040-58-5, 95728-83-9, 104201-66-3, 107468-09-7, 113048-68-3, 116577-12-9]

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 177C.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 174A.
Filler, R. *et al, J. Chem. Eng. Data*, 1964, **9**, 370 (*synth, uv*)
Wittstruck, T.A. *et al, J.A.C.S.*, 1967, **89**, 3803 (*synth, pmr*)
Butt, G. *et al, Spectrochim. Acta A*, 1982, **38**, 301 (*synth, ir, cmr, nitrile*)

3-[4-(Trifluoromethyl)phenyl]-2-propenoic acid, 9CI T-1-00210

4-(Trifluoromethyl)cinnamic acid, 8CI

[2062-26-2]

$C_{10}H_7F_3O_2$ M 216.1

(*E*)-*form* [16642-92-5]
Cryst. Mp 229.5-230°.

(*Z*)-*form* [87212-84-8]
Cryst. Mp 53.0-53.5°.

[20754-22-7, 24654-53-3, 51791-29-8, 57103-25-0, 79947-88-9, 101466-85-7, 101934-50-3, 105919-36-6, 115093-99-7, 120681-07-4, 128408-03-7]

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 179D.
Aldrich Library of NMR Spectra, 2nd edn., **2**, 176B.
Filler, R. *et al, J. Chem. Eng. Data*, 1964, **9**, 370 (*synth, uv*)
Wittstuck, T.A. *et al, J.A.C.S.*, 1967, **89**, 3803 (*synth*)
Galamb, V. *et al, Tet. Lett.*, 1983, **24**, 2965 (*synth, Z-form*)

P-(Trifluoromethyl) phosphonous diamide, 9CI T-1-00211

Diamino(trifluoromethyl)phosphine

$F_3CP(NH_2)_2$

$CH_4F_3N_2P$ M 132.0

N,N,N′,N′-*Tetra-Me:* [3205-96-7].
N,N,N′,N′-*Tetramethyl*-P-(*trifluoromethyl*) *phosphonous diamide*
$C_5H_{12}F_3N_2P$ M 188.1 Liq. Bp_{75} 72°.

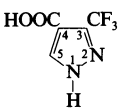
N,N,N′,N′-*Tetra-Et:* [53117-00-3].
N,N,N′,N′-*Tetraethyl*-P-(*trifluoromethyl*) *phosphonous diamide*
$C_9H_{20}F_3N_2P$ M 244.2 Liq. Bp_{19} 93°, $Bp_{2.2}$ 63°.

N,N,N′,N′-*Tetrapropyl:* [53117-01-4].
N,N,N′,N′-*Tetrapropyl*-P-(*trifluoromethyl*) *phosphonous diamide*
$C_{13}H_{28}F_3N_2P$ M 300.3 Liq. Bp_1 79°.

N,N,N′,N′-*Tetrabutyl:* [53117-02-5].
N,N,N′,N′-*Tetrabutyl*-P-(*trifluoromethyl*) *phosphonous diamide*
$C_{17}H_{36}F_3N_2P$ M 356.4 Liq. Bp_1 113°.

Adler, O. *et al, J. Organomet. Chem.*, 1974, **72**, 351 (*synth, ir, pmr*)
Volbach, W. *et al, Tet. Lett.*, 1983, **24**, 5509 (*synth, cmr, F-19 nmr, P-31 nmr*)
Riesel, L. *et al, Z. Anorg. Allg. Chem.*, 1994, **620**, 1099 (*F-19 nmr, P-31 nmr*)

3-Trifluoromethyl-1*H*-pyrazole-4-carboxylic acid T-1-00212



$C_5H_3F_3N_2O_2$ M 180.0

Me ester: [61859-96-9].
$C_6H_5F_3N_2O_2$ M 194.1 Solid ($CHCl_3$). Mp 172-173°.

[155377-19-8]

Saunier, Y.H. *et al, Tetrahedron*, 1976, **32**, 1995 (*Me ester synth, ms, ir, pmr*)
Eur. Pat., 588 357, (1994); *CA*, **121**, 9389h (*Et ester*)

4-Trifluoromethyl-1*H*-pyrazole-3-carboxylic acid T-1-00213

$C_5H_3F_3N_2O_2$ M 180.0

Me ester: [128746-88-3].
$C_6H_5F_3N_2O_2$ M 194.1 Mp 151°.

1H-form

N-*Me, Me ester:* [128746-87-2]. *3-Carbomethoxy-1-methyl-4-(trifluoromethyl) pyrazole*
$C_7H_7F_3N_2O_2$ M 208.1 Mp 89°.

3H-form

N-*Me, Me ester: 5-Carbomethoxy-1-methyl-4-(trifluoromethyl)pyrazole*
$C_7H_7F_3N_2O_2$ M 208.1 No Mp reported.

Tajammal, S. *et al, J. Fluorine Chem.*, 1990, **47**, 45 (*synth, ir, pmr*)
Beagley, B. *et al, Acta Cryst. C*, 1994, **50**, 115 (*cryst struct, deriv*)

5(3)-Trifluoromethyl-1*H*-pyrazole-3(5)-carboxylic acid T-1-00214

[129768-28-1]

$C_5H_3F_3N_2O_2$ M 180.0

Me ester: [19968-13-9].
$C_6H_5F_3N_2O_2$ M 194.1 Mp 134.5-135°.

Et ester: [129768-30-5].
$C_7H_7F_3N_2O_2$ M 208.1 Characterised spectroscopically.

Fields, R. *et al, J.C.S.(C)*, 1968, 1507 (*Me ester, synth, pmr*)
Japan. Pat., 02 129 171, (1990); *CA*, **113**, 172014a (*synth*)
Xu, Y. *et al, Tet. Lett.*, 1992, **33**, 6161 (*Et ester*)

Trifluoro(methyl)sulfur T-1-00215

Updated Entry replacing T-0-04974
Methyl sulfur trifluoride

[65082-47-5]

$MeSF_3$

CH_3F_3S M 104.0
C_s symmetry; $t_{\frac{1}{2}}$ ~15m at r.t. Synth. from MeSCl and AgF_2 in CCl_3F. Unstable at r.t.; can be stored in PTFE at 77K. Reacts with glass, H_2O and air. Sol. CCl_3F (10 g per 100 cm^3 at −23°). Mp −78° to −74°. Bp 80-100°.

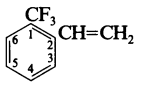
BF_3 complex: see *Difluoro(methyl) sulfonium(1+), D-0-05275*
Tri-deutero compd.: [133377-53-4].
CD_3F_3S M 107.1 Mp −62°.

Gombler, W. *et al, J. Fluorine Chem.*, 1976, **7**, 115.
Downs, A.J. *et al, Inorg. Chem.*, 1989, **28**, 3286 (*ed*)
Downs, A.J. *et al, J.C.S. Dalton*, 1991, 81 (*synth, F-19 nmr, ir, Raman, reactions, deutero deriv*)

1-(Trifluoromethyl)-2-vinylbenzene T-1-00216

1-Ethenyl-2-(trifluoromethyl)benzene, 9CI. 2-Vinylbenzotrifluoride. 2-(Trifluoromethyl) styrene. α,α,α-Trifluoro-2-vinyltoluene

[395-45-9]



$C_9H_7F_3$ M 172.1
d 1.17. Bp_{40} 61°, Bp_{13} 49.5°. n_D^{20} 1.47.

Conciatori, A.B. *et al, J.A.C.S.*, 1950, **72**, 2283 (*synth*)
Brown, H.C. *et al, J.A.C.S.*, 1966, **88**, 5851.
Mesnard, D. *et al, J. Chem. Res., Synop.*, 1981, 270 (*synth*)

1-(Trifluoromethyl)-3-vinylbenzene T-1-00217

1-Ethenyl-3-(trifluoromethyl)benzene, 9CI. 3-(Trifluoromethyl)styrene. α,α,α-Trifluoro-3-vinyltoluene. 3-Vinylbenzotrifluoride

[402-24-4]

$C_9H_7F_3$ M 172.1
d 1.16. Bp_{23} 61-62°.

Conciatori, A.B. *et al, J.A.C.S.*, 1950, **72**, 2283 (*synth*)
Brown, H.C. *et al, J.A.C.S.*, 1966, **88**, 5851 (*synth*)
Trost, B.M. *et al, J.A.C.S.*, 1973, **95**, 5288 (*synth, ir, pmr*)
Mesnard, D. *et al, J. Chem. Res., Synop.*, 1981, 270 (*synth*)
Happer, D.A.R., *J.C.S. Perkin 2*, 1984, 1673 (*cmr*)

1-(Trifluoromethyl)-4-vinylbenzene T-1-00218

1-Ethenyl-4-(trifluoromethyl)benzene, 9CI. 4-(Trifluoromethyl)styrene. α,α,α-Trifluoro-4-vinyltoluene. 4-Vinylbenzotrifluoride

[402-50-6]

$C_9H_7F_3$ M 172.1
d 1.16. Bp_{27} 69°, Bp_{14} 38°.

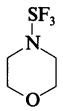
[97552-17-5, 97552-18-6]

Conciatori, A.B. *et al, J.A.C.S.*, 1950, **72**, 2283 (*synth*)
Brown, H.C. *et al, J.A.C.S.*, 1966, **88**, 5851.
Hamer, G.K. *et al, Can. J. Chem.*, 1973, **51**, 897 (*pmr, cmr*)
Mesnard, D. *et al, J. Chem. Res., Synop.*, 1981, 270 (*synth*)
Happer, D.A.R., *J.C.S. Perkin 2*, 1984, 1673 (*cmr*)
Abdel-Baky, S. *et al, Synth. Commun.*, 1988, **18**, 1795 (*synth*)

Trifluoro(morpholinato-N^4)sulfur, 9CI T-1-00219

Morpholinosulfur trifluoride. Morph-DAST

[51010-74-3]



$C_4H_8F_3NOS$ M 175.1
Fluorinating agent. Liq. d 1.44. $Bp_{0.5}$ 41-42°. n_D^{20} 1.4545.

Markovskii, L.N. *et al, Synthesis*, 1973, 787 (*synth, use*)

1,1,1-Trifluoro-3-phenylpropane T-1-00220

(3,3,3-Trifluoropropyl)benzene, 9CI

[1579-80-2]

$PhCH_2CH_2CF_3$

$C_9H_9F_3$ M 174.1
Bp 155-157°.

Takusari, H. *et al, Chem. Lett.*, 1984, 885.
Kobayashi, Y. *et al, Chem. Pharm. Bull.*, 1984, **32**, 4382.

1,1,1-Trifluoro-3-phenyl-2-propanone T-1-00221

Benzyl trifluoromethyl ketone

[350-92-5]

$PhCH_2COCF_3$

$C_9H_7F_3O$ M 188.1
Liq. Bp_{15} 72-75°. n_D^{25} 1.4432.

Oxime:
$C_9H_8F_3NO$ M 203.1 Mp 40-42°. Bp_3 91-92°.

Semicarbazone: Needles (MeOH aq.). Mp 129-130°.

[125774-47-2, 125774-52-9]

Nes, W.R. *et al, J.A.C.S.*, 1950, **72**, 5409 (*synth, derivs*)
Begue, J.P. *et al, J. Fluorine Chem.*, 1988, **39**, 271 (*synth*)
Quinze, K. *et al, J. Fluorine Chem.*, 1989, **44**, 211 (*bibl, synth, ir, pmr, cmr*)

3,3,3-Trifluoro-2-phenylpropene T-1-00222

[1-(Trifluoromethyl)ethenyl]benzene, 9CI. α-(Trifluoromethyl)styrene

[384-64-5]

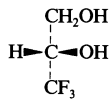
$H_2C{=}CPhCF_3$

$C_9H_7F_3$ M 172.1
Oil. d_4^{21} 1.17. Bp 148-148.5°. n_D^{21} 1.4603.

Tarrant, P. *et al, J.O.C.*, 1959, **24**, 238 (*synth*)

3,3,3-Trifluoro-1,2-propanediol T-1-00223

[431-39-0]



(*S*)-*form*

$C_3H_5F_3O_2$ M 130.0

(S)-form [148683-14-1]
Liq. Bp_{25} 100° (Kugelrohr). $[\alpha]_D^{24}$ −10.95 (c, 1.4 in MeOH) (96% ee).

1-Et ether: [160595-65-3]. *1-Ethoxy-2,2,2-trifluoroethanol*
$C_5H_9F_3O_2$ M 158.1 Liq. Bp_{40} 100° (Kugelrohr). $[\alpha]_D^{22}$ −11.20 (c, 1.4 in MeOH).

(±)-form
Viscous liq. with tendency to supercool. d_{20}^{20} 1.151. Mp 25.3°. Bp_{26} 88.6°, Bp_{10} 69.5-70.1°. n_D^{20} 1.3617.

α-Naphthylurethane: Cryst. solid. Mp 198-199°.

McBee, E.T. *et al, J.A.C.S.*, 1952, **74**, 3022 (*synth*)
Ramachandran, P.V. *et al, J.O.C.*, 1995, **60**, 41 (*synth, ir, pmr, cmr, F-19 nmr*)

2,2,2-Trifluoro-3′-(trifluoromethyl)acetophenone T-1-00224

2,2,2-Trifluoro-1-[3-(trifluoromethyl)phenyl] ethanone, 9CI. 1-(Trifluoroacetyl)-3-(trifluoromethyl)benzene

[721-37-9]

$C_9H_4F_6O$ M 242.1
Liq. d 1.42. Bp_{24} 65-67°.

Fuchs, R. *et al, J.O.C.*, 1957, **22**, 993 (*synth*)
Liu, K.T. *et al, J. Phys. Org. Chem.*, 1989, **2**, 363 (*synth, O-17 pmr*)

2,2,2-Trifluoro-4′-(trifluoromethyl) acetophenone T-1-00225

2,2,2-Trifluoro-1-[4-(trifluoromethyl)phenyl] ethanone, 9CI. 1-(Trifluoroacetyl)-4-(trifluoromethyl)benzene

[74853-66-0]

$C_9H_4F_6O$ M 242.1
Liq. Bp_{15} 63-65°.

Creary, X., *J.O.C.*, 1987, **52**, 5026 (*synth, ir, pmr*)
Liu, K.T. *et al, J. Phys. Org. Chem.*, 1989, **2**, 363 (*synth, O-17 nmr*)

Trifluoro(trifluoromethyl) sulfur T-1-00226

Updated Entry replacing T-0-05049
Trifluoromethylsulfur trifluoride

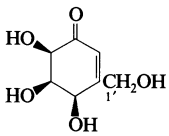
[374-10-7]

F_3CSF_3

CF_6S M 158.0
Interatomic distances: S—F_{eq} 156.5, S—F_{ax} 165.5, S—C 188.7 pm; angles: $F_{eq}SF_{ax}$ 86.1°, CSF_{ax} 86.5°, $F_{eq}SC$ 98.4°. Synth. from CS_2 or CF_3SSCF_3 + AgF_2 at −50°. Colourless gas. Bp −7°.

Tyczkowski, E.A. *et al, J.A.C.S.*, 1953, **75**, 3523.
Sheppard, W.A., *J.A.C.S.*, 1962, **84**, 3058 (*synth, reactions*)
Lawless, E.W. *et al, Inorg. Chem.*, 1968, **7**, 391 (*synth, F-19 nmr, ir*)
Minkwitz, R. *et al, J. Fluorine Chem.*, 1987, **37**, 397 (*reactions*)
Minkwitz, R. *et al, Inorg. Chem.*, 1992, **31**, 2104 (*ed*)

4,5,6-Trihydroxy-3-(hydroxymethyl)-2-cyclohexen-1-one T-1-00227



(4*R**,5R*,6R*)-*form*

$C_7H_{10}O_5$ M 174.1

(4R*,5R*,6R*)-form [148154-54-5] ***Gabosine J***
Prod. by *Streptomyces kurssanovii.*

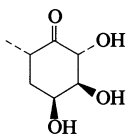
(4R*,5S*,6R*)-form [148099-41-6] ***Gabosine I***
Prod. by *S. kurssanovii.* Mp 128-129°. $[\alpha]_D^{20}$ −61.4 (c, 1 in MeOH).

1′-O-Ac: [127545-54-4]. ***Gabosine G***
$C_9H_{12}O_6$ M 216.1 Prod. by *S. chromofuscus.*

1′-Deoxy: [127545-55-5]. *4,5,6-Trihydroxy-3-methyl-2-cyclohexen-1-one.* ***Gabosine H***
$C_7H_{10}O_4$ M 158.1 Prod. by *S. chromofuscus.* Cryst. Mp 123°. $[\alpha]_D^{20}$ −68.3 (c, 0.58 in MeOH).

Bach, G. *et al, Annalen*, 1993, 241 (*isol, pmr, cmr*)

2,3,4-Trihydroxy-6-methylcyclohexanone T-1-00228



(2*R*,3*S*,4*S*,6*S*)-*form*

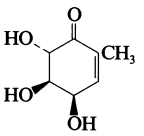
$C_7H_{12}O_4$ M 160.1

(2R,3S,4S,6S)-form [127707-32-8] ***Gabosine F***
Prod. by *Streptomyces cellulosae* subsp. *griseorubiginosus.* Mp 82-85°. $[\alpha]_D^{20}$ +94 (c, 1 in MeOH).

(2S,3R,4R,6R)-form [106750-01-0] ***Gabosine B***
Prod. by *S. cellulosae* subsp. *griseorubiginosus.* Mp 88°. $[\alpha]_D^{20}$ −106 (c, 0.45 in MeOH).

Mueler, A. *et al, Helv. Chim. Acta*, 1986, **69**, 1829 (*synth*)
Bach, G. *et al, Annalen*, 1993, **24**, 1 (*isol, pmr, cmr*)

4,5,6-Trihydroxy-2-methyl-2-cyclohexen-1-one T-1-00229



$C_7H_{10}O_4$ M 158.1

(4R,5R,6S)-form [127545-53-3] ***Gabosine A***
Prod. by *Streptomyces cellulosae* subsp. *griseorubiginosus.* Cryst. $[\alpha]_D^{20}$ −132 (c, 1 in MeOH).

Bach, G. *et al, Annalen*, 1993, 241 (*isol, pmr, cmr*)

4,5,7-Trihydroxy-2-naphthalenecarboxylic acid T-1-00230

$C_{11}H_8O_5$ M 220.1

5,7-Di-Me ether: [77729-57-8]. *4-Hydroxy-5,7-dimethoxy-2-naphthalenecarboxylic acid*
$C_{13}H_{12}O_5$ M 248.2 Prisms (EtOH). Mp 245-247°.

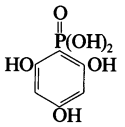
5,7-Di-Me ether, Me ester: [78395-68-3].
$C_{14}H_{14}O_5$ M 262.2 Needles (EtOH). Mp 160-161° (149-151°).

5,7-Di-Me ether, 4-Ac, Me ester: [77729-56-7].
$C_{16}H_{16}O_6$ M 304.2 Needles (EtOH or MeOH). Mp 153-154°.

Tri-Me ether, Me ester: [74694-98-7].
$C_{15}H_{16}O_5$ M 276.2 Prisms (EtOH). Mp 145-146°.

Cameron, D.W. *et al, Aust. J. Chem.*, 1980, **33**, 2531 (*5,7-di-Me ether, tri-Me ether*)
Liu, J. *et al, Synthesis*, 1995, 914 (*5,7-di-Me ether*)

(2,4,6-Trihydroxyphenyl) phosphonic acid T-1-00231



$C_6H_7O_6P$ M 206.0

2,4-Di-Me ether: [136829-82-8]. *(2-Hydroxy-4,6-dimethoxyphenyl)phosphonic acid*
$C_8H_{11}O_6P$ M 234.1 Solid. Mp 128-129°.

2,4-Di-Me ether, Et ester: [80615-42-5]. *Diethyl (2-hydroxy-4,6-dimethoxyphenyl) phosphonate*
$C_{10}H_{15}O_6P$ M 262.1 Liq. $Bp_{0.05}$ 137-141°.

*2,4-Di-Me ether, di-*tert*-butyl ester:* [136829-80-6]. *Bis(1,1-dimethylethyl) (2-hydroxy-4,6-dimethoxyphenyl)phosphonate*
$C_{16}H_{27}O_6P$ M 346.3 Cryst. (CH_2Cl_2/petrol). Mp 115-116°.

2,4-Di-Me ether, bis(dimethylamide): P-(*2-Hydroxy-4,6-dimethoxyphenyl*)-N,N,N′,N′-*tetramethylphosphonic diamide*
$C_{12}H_{21}N_2O_4P$ M 288.2 Cryst. (Et_2O/hexane). Mp 89-91°.

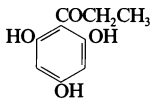
Melvin, L.S., *Tet. Lett.*, 1981, **22**, 3375.
Watanabe, M. *et al, Chem. Pharm. Bull.*, 1990, **38**, 2637 (*amide, synth, ir, uv, pmr*)

Dhawan, B. *et al, Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, **61**, 183 (*synth, ester, pmr, cmr, P-31 nmr*)

1-(2,4,6-Trihydroxyphenyl)-1-propanone, 9CI T-1-00232

2',4',6'-Trihydroxypropiophenone. ***Flopropione, INN.*** *Phloropropiophenone. Fluropropiophenone. Compacsul. Cospanon. Ecapron. Pellegal. Argobyl. Floveton. Saritron. Spamorin. Labrodax. Tryalon. Mirulevatin. Padeskin. Profenon†*

[2295-58-1]



$C_9H_{10}O_4$ M 182.1

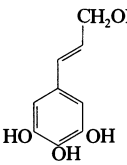
Constit. of *Inula viscosa*. 5-HT_{1A} receptor antagonist, spasmolytic agent. Needles + $1H_2O$ (H_2O). Sl. sol. H_2O. Mp 175-176°.

▶ LD_{50} (rat, orl) 2380 mg/kg. LD_{50} (rat, ivn) 246 mg/kg. UH4429100.

Howells, H.P. *et al, J.A.C.S.*, 1932, **54**, 2451 (*synth*)
Populaire, P. *et al, Therapie*, 1968, **23**, 91 (*metab*)
Inoue, S., *Jpn. J. Pharmacol.*, 1969, **19**, 224 (*pharmacol*)
Mizobuchi, S. *et al, Agric. Biol. Chem.*, 1985, **49**, 719 (*synth*)
Bolte, M.L. *et al, Agric. Biol. Chem.*, 1985, **49**, 761 (*synth*)
Grande, M. *et al, Planta Med.*, 1985, 414 (*isol*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 1371.
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 7th edn., Akademie-Verlag, Berlin, 1994, 1432 (*synonyms*)

3-(3,4,5-Trihydroxyphenyl)-2-propen-1-ol T-1-00233

3',4',5'-Trihydroxycinnamyl alcohol



$C_9H_{10}O_4$ M 182.1

(E)-form

Mp 167°. Probable (*E*)-config. assumed here.

3',4',5'-Tri-Me ether: [30273-62-2]. *3',4',5'-Trimethoxycinnamyl alcohol*
$C_{12}H_{16}O_4$ M 224.2 Constit. of *Myristica fragrans* and other plant spp. including *Asia sarum* sp. *Cineraria fruticulorum* and *Uvariodendron connivens*. Mp 110°. $Bp_{0.15}$ 145-147°.

3',4',5'-Tri-Me ether, Ac: [87200-84-8].
$C_{14}H_{18}O_5$ M 266.2 Constit. of oil of bergamot (*Citrus bergamia*). Oil.

3-Me, 4,5-methylene ether: [69618-94-6]. *3-(3-Methoxy-4,5-methylenedioxyphenyl)-2-propen-1-ol. 3'-Methoxy-4',5'-methylenedioxycinnamyl alcohol*
$C_{11}H_{12}O_4$ M 208.2 Constit. of *M. fragrans*. Needles (EtOAc/hexane). Mp 72-73°.

3',4',5'-Tri-Me ether, O-(3-methylbutanoyl): [105072-20-6]. *3,4,5-Trimethoxycinnamyl isovalerate*
$C_{17}H_{24}O_5$ M 308.3 Constit. of the leaves of *Juniperus thurifera*. Oil.

3',4',5'-Tri-Me ether, 1-O-β-D-glucopyranoside: [135743-09-8]. ***Icariside H_1***
$C_{18}H_{26}O_9$ M 386.3 Constit. of *Epimedium sagittatum*. Amorph. powder. $[\alpha]_D^{23}$ −47.6 (c, 0.62 in MeOH).

(Z)-form

3',4',5'-Tri-Me ether: [30273-66-6]. Pale yellow oil. $Bp_{0.25}$ 138-140°.

[1504-56-9, 30273-66-6, 97094-25-2]

Freudenberg, K. *et al, Chem. Ber.*, 1953, **86**, 190; 1955, **88**, 16 (*synth*)
Cooper, P.D. *et al, Can. J. Chem.*, 1970, **48**, 3882 (*synth*)
Kato, M. *et al, Bull. Chem. Soc. Jpn.*, 1974, **47**, 1516 (*deriv, synth*)
Ehret, C. *et al, Phytochemistry*, 1982, **21**, 2984 (*isol, deriv, Ac*)
Mohammed, I. *et al, J. Nat. Prod.*, 1985, **48**, 328 (*isol, pmr, cmr*)
San Feliciano, A. *et al, J. Nat. Prod.*, 1986, **49**, 677 (*isol, deriv*)
Ponpipom, M.M. *et al, J. Med. Chem.*, 1987, **30**, 136 (*synth*)
Hattori, M. *et al, Chem. Pharm. Bull.*, 1988, **36**, 648 (*isol*)
Matsushita, H. *et al, Phytochemistry*, 1991, **30**, 2025 (*Icariside H_1*)

Triiodoethene, 9CI T-1-00234

Triiodoethylene

[10065-29-9]

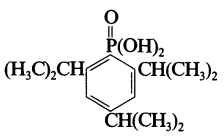
$ICH{=}CI_2$

C_2HI_3 M 405.7
Yellow oil.

Krikorian, S.E. *et al, J.O.C.*, 1994, **59**, 3742 (*synth, ir, pmr, ms*)

(2,4,6-Triisopropylphenyl) phosphonic acid, 8CI T-1-00235

[2,4,6-Tris(1-methylethyl)phenyl]phosphonic acid, 9CI



$C_{15}H_{25}O_3P$ M 284.3

Dichloride: [114070-56-3].
$C_{15}H_{23}Cl_2OP$ M 321.2 Solid. V. sp. sol. in petrol. Mp 108-112°.

Freeman, S. *et al, J.C.S. Perkin 1*, 1987, 1399 (*synth, ir, pmr, P-31 nmr*)

Trimethylarsine, 9CI T-1-00236

Arsenic trimethyl. Gosio gas

[593-88-4]

$AsMe_3$

C_3H_9As M 120.0

Metab. prod. from microbial action on many arsenicals. Found in v. low levels in some species of deep-sea crustaceans. Ligand for most heavy metals. Liq. with unpleasant penetrating odour. Mp 55°.

Complexes readily with BH_3 and B trihalides; also with As, and Sb halides, (inorganic and organic). Absorbs O_2 from air → Trimethylarsine oxide, T-0-05474.

▶ Highly toxic. Spontaneously flammable in air. CH8800000.

Oxide: see *Trimethylarsine oxide, T-0-05474*
Sulfide: see *Trimethylarsine sulfide, T-0-05476*
Selenide: see *Trimethylarsine selenide, T-0-05475*
Chlorine complex (1:1): see *Dichlorotrimethylarsorane, D-0-04560*
Bromine complex (1:1): see *Dibromotrimethylarsorane, D-0-02902*
BBr_3 complex (1:1): [52827-82-4].
$C_3H_9AsBBr_3$ M 370.5 Solid. Mp 245°.

BI_3 complex (1:1): [55042-21-2].
$C_3H_9AsBI_3$ M 511.5 Solid. Mp 274-275°. Slowly dec. in $CHCl_3$ → $Me_3AsI^{\oplus}I^{\ominus}$.

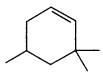
AsI_3 complex (1:1): [26459-38-1].
$C_3H_9As_2I_3$ M 575.6 Solid. Mp 140-144° dec.

Summers, J.C. *et al, Inorg. Chem.*, 1970, **9**, 862 (*complexes*)
Svergun, V.I. *et al, Izv. Akad. Nauk SSSR, Ser. Khim.*, 1970, 482; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1970, 442 (*nqr*)
Kostyanovskii, R.G. *et al, Org. Mass Spectrom.*, 1972, **6**, 1183 (*ms*)
Fournier, L. *et al, Synth. React. Inorg. Met.-Org. Chem.*, 1972, **2**, 53 (*synth*)
Dewar, M.I.S. *et al, J.C.S. Dalton*, 1973, 2381 (*As-75 nmr*)
Durig, J.R. *et al, Inorg. Chem.*, 1974, **13**, 2306 (*ir, Raman, microwave, BH_3 complex*)
Durand, M. *et al, J. Chim. Phys. Phys.-Chim. Biol.*, 1974, **71**, 847 (*pmr*)
Denniston, M.L. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 2175 (*B complexes, pmr, B-11 nmr*)
Elbel, S. *et al, J.C.S. Faraday 2*, 1974, **70**, 555 (*pe*)
Baliman, G. *et al, Helv. Chim. Acta*, 1975, **58**, 1913 (*cmr*)
Mente, D.C. *et al, Inorg. Chem.*, 1975, **14**, 1862 (*B complexes, ir, Raman, ms*)
Efremov, E.A. *et al, Zh. Fiz. Khim.*, 1975, **49**, 1844; *CA*, **83**, 183571.
Rojhantalab, H. *et al, Spectrochim. Acta A*, 1976, **32**, 947 (*ir, Raman*)
Beagley, B. *et al, J. Mol. Struct.*, 1977, **38**, 229 (*struct*)
Durand, M. *et al, J.C.S. Dalton*, 1977, **37**, 57 (*B complexes, pmr, B-11 nmr*)
Apel, J. *et al, Z. Anorg. Allg. Chem.*, 1979, **453**, 28 (*nmr*)
Gushikem, Y. *et al, J.C.S. Dalton*, 1980, 2016 (*B complexes, ir, Raman*)
McKean, D.C. *et al, Spectrochim. Acta A*, 1982, **38**, 113 (*ir*)
Blom, R. *et al, Acta Chem. Scand., Ser. A*, 1983, **37**, 595 (*ed, struct*)
Gleiter, R. *et al, Chem. Ber.*, 1983, **116**, 3745 (*pe*)
Whitfield, F.B. *et al, Chem. Ind.* (*London*), 1983, 786 (*isol*)
Edmonds, J.S. *et al, J.C.S. Perkin 1*, 1983, 2375 (*pmr, cmr*)
Chadha, R.K. *et al, J. Crystallogr. Spectrosc. Res.*, 1985, **15**, 53 (*B complexes, cryst struct*)
Chehaybar, J.M. *et al, Inorg. Chim. Acta*, 1986, **112**, 209 (*B complexes, pmr, B-11 nmr*)
Fischer, M. *et al, Chemtronics*, 1988, **3**, 156 (*uv*)
Organomet. Synth., 1988, **4**, 582 (*synth*)
Ismail, K. *et al, Pertanika J. Trop. Agric. Sci.*, 1988, **11**, 437 (*synth*)

Watkins, C.L. *et al*, *Magn. Reson. Chem.*, 1989, **27**, 616 (*pmr, cmr*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, TLH150.
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworth, London and Boston, 1990, 396.

3,3,5-Trimethylcyclohexene, 9CI, 8CI T-1-00237

[503-45-7]



C_9H_{16} M 124.2

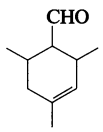
(±)-*form*
Mp −85.4°. Bp 131.5°.

Trachtenberg, E.N. *et al*, *J.O.C.*, 1970, **35**, 1653 (*synth, ir*)
Barillier, D. *et al*, *Tetrahedron*, 1983, **39**, 767 (*cmr*)

2,4,6-Trimethyl-3-cyclohexene-1-carboxaldehyde T-1-00238

2,4,6-Trimethyl-Δ³-tetrahydrobenzaldehyde. Isocyclocitral

[1335-66-6]



$C_{10}H_{16}O$ M 152.2
Used in perfumery. d 0.92. Bp_{16} 85-90°. Mixt. of stereoisomers.

Semicarbazone: Mp 182-183°.

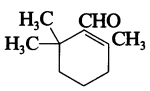
[1423-46-7]

Diels, O. *et al*, *Annalen*, 1929, **470**, 62 (*synth*)
Dupont, G. *et al*, *Bull. Soc. Chim. Fr.*, 1939, **6**, 1208 (*synth*)
Nazarov, I.N. *et al*, *Zh. Obshch. Khim.*, 1958, **28**, 3061; *CA*, **53**, 10069h (*synth*)

2,6,6-Trimethyl-1-cyclohexene-1-carboxaldehyde, 9CI, 8CI T-1-00239

β-Cyclocitral

[432-25-7]



$C_{10}H_{16}O$ M 152.2
Bp_{25} 105°, Bp_{15} 94-97°.

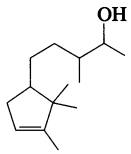
2,4-Dinitrophenylhydrazone: [14186-18-6]. Mp 172°.

Bohlmann, F. *et al*, *Org. Magn. Reson.*, 1975, **7**, 426.
Das, P.K. *et al*, *J. Phys. Chem.*, 1978, **82**, 2081 (*uv*)
Cainelli, G. *et al*, *J.C.S. Perkin 1*, 1979, 1597 (*synth, ir, pmr*)
Jalali-Naini, M. *et al*, *Tetrahedron*, 1983, **39**, 749 (*synth, ir, pmr*)

5-(2,2,3-Trimethyl-3-cyclopentenyl)-3-methyl-2-pentanol T-1-00240

α,β,2,2,3-Pentamethyl-3-cyclopentene-1-butanol, 9CI. Sandalone

[65113-99-7]



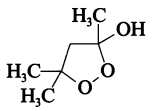
$C_{14}H_{26}O$ M 210.3
Used in perfumery. Liq. with sweet, woody sandalwood type odour. d 0.90.

Swiss Pat., 629 462, (1982); *CA*, **97**, 198415h.
Swiss Pat., 629, 461, (1982); *CA*, **97**, 198416j.

3,5,5-Trimethyl-1,2-dioxolan-3-ol, 8CI T-1-00241

Diolan

[27779-47-1]



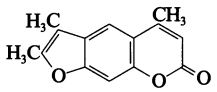
$C_6H_{12}O_3$ M 132.1

[19789-15-2]

Gibson, D.H. *et al*, *Tet. Lett.*, 1969, 2203 (*synth, pmr*)

2,3,5-Trimethyl-7*H*-furo[3,2-*g*][1]benzopyran-7-one T-1-00242

[13008-11-2]



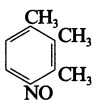
$C_{14}H_{12}O_3$ M 228.2
Mp 189°.

Royer, R. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 1716 (*synth*)
Adam, W. *et al*, *Annalen*, 1990, 1227 (*cmr, pmr*)

1,2,3-Trimethyl-4-nitrosobenzene T-1-00243

4-Nitrosolemimellitene

[158815-54-4]



$C_9H_{11}NO$ M 149.1
Cryst. (MeOH). Mp 79-80°.

Bosch, E. *et al*, *J.O.C.*, 1994, **59**, 5573 (*synth, ir, pmr, cmr*)

1,2,4-Trimethyl-5-nitrosobenzene, 9CI T-1-00244

5-Nitrosopseudocumene

[158815-55-5]

$C_9H_{11}NO$ M 149.1
Green cryst. (CH_2Cl_2), cryst. (MeOH). Mp 43-44° (from CH_2Cl_2), Mp 62-63° (from MeOH).

Bamberger, E., *Ber.*, 1910, **43**, 1842.
Bosch, E. *et al*, *J.O.C.*, 1994, **59**, 5573 (*synth, ir, pmr, cmr*)

Trimethyloctadecylammonium(1+), 8CI T-1-00245

N,N,N-*Trimethyloctadecanaminium, 9CI*

[15461-40-2]

$H_3C(CH_2)_{17}N^{\oplus}Me_3$

$C_{21}H_{46}N^{\oplus}$ M 312.6 (ion)

Chloride: [112-03-8].
Trimethyloctadecylammonium chloride. Boraquat P30
$C_{21}H_{46}ClN$ M 348.0 Surfactant. Used. in cosmetics. Cryst. Mp 220° dec.

Bromide: [1120-02-1].
$C_{21}H_{46}BrN$ M 392.5 Cryst. (EtOH). Mp 250° dec.

Iodide: [4292-25-5].
$C_{21}H_{46}IN$ M 439.5 Cryst. Mp 227-230°.

Baltzly, R. *et al*, *J.A.C.S.*, 1942, **64**, 2514 (*iodide*)
Shelton, R.S. *et al*, *J.A.C.S.*, 1946, **68**, 753 (*bromide*)
Celia, J.A. *et al*, *J.A.C.S.*, 1952, **74**, 2061 (*chloride*)
Sprintschnik, G. *et al*, *J.A.C.S.*, 1977, **99**, 4947 (*bromide*)
Isa, K. *et al*, *Org. Mass Spectrom.*, 1983, **18**, 229 (*ms*)

N,N,N-Trimethyl-2-oxoethanaminium(1+), 9CI T-1-00246

(Formylmethyl)trimethylammonium, 8CI. (Trimethylammonio)acetaldehyde. Betaine aldehyde

[7418-61-3]

$Me_3N^{\oplus}CH_2CHO$

$C_5H_{12}NO^{\oplus}$ M 102.1 (ion)
Choline metabolite.

Chloride: [92397-80-3].
$C_5H_{12}ClNO$ M 137.6 Cryst. + H_2O. Mp 142-144° (123-124°).

Tetrachloroaurate: Cryst. (HCl). Mp 215-217°.

2,4-Dinitrophenylhydrazone, picrate, chloride: Yellow cryst. Mp 181-183°.

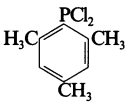
Di-Et acetal, bromide:
$C_9H_{22}BrNO_2$ M 256.1 Cryst. ($EtOH/Et_2O$). Mp 150-152°.

Mann, P.J.G. *et al*, *Biochem. J.*, 1937, **31**, 869 (*aurate*)
Bergel, F. *et al*, *J.C.S.*, 1950, 1439 (*bromide*)
Jellinek, M. *et al*, *J. Biol. Chem.*, 1959, **234**, 1171 (*chloride*)
Gorham, J. *et al*, *J. Chromatogr.*, 1985, **350**, 245 (*hplc*)
Tokmakjian, S.D. *et al*, *Biochem. Int.*, 1989, **18**, 751 (*occur*)
Fortier, G. *et al*, *Anal. Lett.*, 1990, **23**, 1607 (*anal*)

(2,4,6-Trimethylphenyl) phosphonous dichloride, 9CI T-1-00247

Mesitylphosphonous dichloride, 8CI. Dichloromesitylphosphine

[6781-96-0]



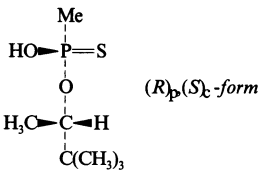
$C_9H_{11}Cl_2P$ M 221.0

Liq. which slowly cryst. Bp_2 145-150°.

Goldwhite, H. *et al, J. Organomet. Chem.*, 1986, **310**, 21 (*synth, P-31 nmr*)
Bentrude, W.S. *et al, J.A.C.S.*, 1988, **110**, 7119 (*synth, P-31 nmr*)
Goede, S.J. *et al, Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1994, **113**, 278 (*P-31 nmr*)

O-(1,2,2-Trimethylpropyl) methylphosphonothioate T-1-00248

O-*Pinacolyl methylphosphonothioate*



$(R)_P(S)_C$-*form*

$C_7H_{17}O_2PS$ M 196.2

(R)p(S)c-form

(R)-*1-Phenylethylamine salt:* Cryst. $[\alpha]_D$ +13.8 (c, 1.2 in MeOH).

(S)p(S)c-form

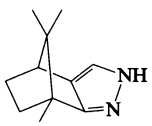
(S)-*1-Phenylethylamine salt:* Cryst. $[\alpha]_D$ −4.2 (c, 0.8 in MeOH).

[103730-70-7, 103773-68-8, 116498-76-1, 116498-78-3]

Hall, C.R. *et al, Tetrahedron*, 1985, **41**, 4909 (*synth, resoln, pmr, P-31 nmr*)
Fentiman, A.F., *CA*, 1988, **109**, 149622.

7,8,8-Trimethyl-4,5,6,7-tetrahydro-4,7-methano-1(2*H*)-indazole, 9CI T-1-00249

Campho[2,3-c]pyrazole



$C_{11}H_{16}N_2$ M 176.2

(+)-form [65529-87-5]

Readily prepd. from camphor. Used in chiral homogeneous catalysis. Cryst. (petrol). Mp 153-155° (144-145°). $[\alpha]_D^{25}$ +42.7 (c, 0.234 in EtOH), $[\alpha]_D^{25}$ +33.2 (c, 1 in $CHCl_3$).

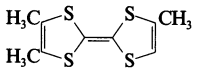
[56655-93-7, 72345-25-6, 147383-60-6]

Nagai, S. *et al, Chem. Pharm. Bull.*, 1979, **27**, 1771 (*synth, pmr*)
Brunner, H. *et al, Chem. Ber.*, 1992, **125**, 701 (*synth, ir, pmr, ms*)
Llamas-Saiz, A.L. *et al, Acta Cryst. C*, 1993, **49**, 724 (*cryst struct, cmr, bibl*)
Le Cloux, D.D. *et al, Organometallics*, 1994, **13**, 2855 (*synth*)

Trimethyltetrathiafulvalene T-1-00250

4,5-Dimethyl-2-(4-methyl-1,3-dithiol-2-ylidene)-1,3-dithiole, 9CI. Trimethyl-1,3-dithiol-2-ylidene

[49868-52-2]

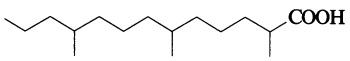


$C_9H_{10}S_4$ M 246.4

Forms radical cation salts of high conductivity. Orange needles (MeCN). Mp 110° (103-104°).

Mora, H. *et al, Bull. Soc. Chim. Belg.*, 1992, **101**, 137 (*synth, pmr*)
Dolbecq, A. *et al, Chem. Mater.*, 1994, **6**, 1413 (*synth, pmr*)
Moore, A.J. *et al, Synthesis*, 1995, 675 (*synth, pmr, uv*)

2,6,10-Trimethyltridecanoic acid T-1-00251



$C_{16}H_{32}O_2$ M 256.4

Me ester: [155450-29-6].
$C_{17}H_{34}O_2$ M 270.4 Major component of the pheromone prod. by the male stink bugs *Euschistus heros* and *E. obscurus*. Oil. All 8 stereoisomers have been synth. but stereochem. of nat. prod. not yet determined (1994).

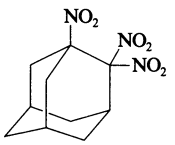
[161905-42-6, 161905-43-7, 161905-44-8, 161905-45-9, 161905-46-0, 161905-47-1, 161905-48-2, 161905-49-3, 161905-50-6, 161905-51-7, 161905-52-8, 161905-53-9, 161905-54-0, 161905-55-1, 161905-56-2, 161905-57-3]

Mori, K. *et al, Annalen*, 1994, 637, 1153 (*synth, pmr, cmr*)

1,2,2-Trinitroadamantane T-1-00252

1,2,2-Trinitrotricyclo[3.3.1.1^{3,7}]decane, 9CI

[162710-74-9]



$C_{10}H_{13}N_3O_6$ M 271.2

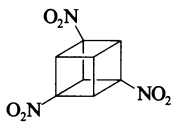
Cryst. (Me_2CO/hexane). Mp 248-249°.

Dave, P.R. *et al, J.O.C.*, 1995, **60**, 1895 (*synth, ir, pmr, cmr*)

1,3,5-Trinitrocubane T-1-00253

1,3,5-Trinitropentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}] octane, 9CI

[99393-49-4]



$C_8H_5N_3O_6$ M 239.1

Solid. Mp 250° dec.

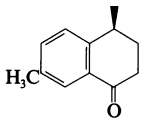
▶ Potentially explosive.

Eaton, P.E. *et al, J.A.C.S.*, 1993, **115**, 10195 (*synth, pmr, cmr, ir, cryst struct, haz*)

11,12,13-Trinor-7-calamenone T-1-00254

3,4-Dihydro-4,7-dimethyl-1(2H)naphthalenone. 4,7-Dimethyltetralone

[28449-86-7]



(*S*)-*form*

$C_{12}H_{14}O$ M 174.2

(S)-form [155748-76-8]

Constit. of *Siparuna macrotepala* and oil of lavender.

(±)-form [85867-62-5]

Liq. Bp_6 129°, $Bp_{0.8}$ 106.5-108°.

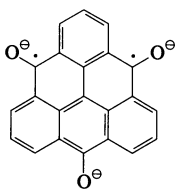
2,4-Dinitrophenylhydrazone: [74285-39-5]. Red cryst. (EtOAc/$CHCl_3$). Mp 244-244.3°.

Semicarbazone: Needles (EtOH). Mp 196-197°.

[74285-39-5]

Johnson, W.S. *et al, J.A.C.S.*, 1947, **69**, 792 (*synth*)
Phillips, D.D., *J.A.C.S.*, 1955, **77**, 3658 (*synth*)
Kaiser, R. *et al, Helv. Chim. Acta*, 1983, **66**, 1843 (*isol*)
El-Seedi, H. *et al, Phytochemistry*, 1994, **35**, 1495 (*isol, pmr, cmr*)

4,8,12-Trioxodibenzo[*cd,mn*] pyrenediyl(3−) T-1-00255



$C_{22}H_9O_3^{3\ominus}$ M 321.3 (ion)

First deriv. of the ground-state biradical ring system Triangulene, T-1-00143. Brown-green in soln. Stable for many months *in vacuo*, instantly dec. by O_2.

Allinson, G. *et al, J.C.S. Perkin 1*, 1995, 385 (*synth, esr*)

Triphenylbis(phenylethynyl) phosphorane, 9CI T-1-00256

[147437-84-1]

$PhC{\equiv}CPPh_3C{\equiv}CPh$

$C_{34}H_{25}P$ M 464.5

Milky cryst. Mp 45-65° dec. With H_2O → $PhC{\equiv}CH$ + Ph_3PO. When heated → Ph_3P + Ph_3PO + $PhC{\equiv}CC{\equiv}CPh$.

Ogawa, S. *et al, Tet. Lett.*, 1993, **34**, 838 (*synth, ms, pmr, cmr, P-31 nmr, props*)

1,1,4-Triphenyl-1-buten-3-yne T-1-00257

1,1',1''-(1-Buten-3-yn-4-yl-1-ylidene) trisbenzene, 9CI

[59277-58-6]

$Ph_2C{=}CHC{\equiv}CPh$

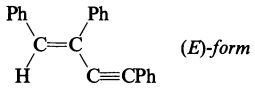
$C_{22}H_{16}$ M 280.3

Cryst. (EtOH). Mp 104-105°.

Marcuzzi, F. *et al, J.C.S. Perkin 1*, 1993, 2957 (*synth, ir, pmr*)

1,2,4-Triphenyl-1-buten-3-yne T-1-00258

1,1′,1″-(1-Buten-3-yne-1,2,4-triyl)trisbenzene, 9CI



(*E*)-form

$C_{22}H_{16}$ M 280.3

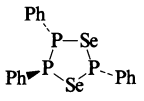
(***E*)-form** [154617-23-9]
Cryst. (EtOH). Mp 49-50°.

(***Z*)-form** [62677-52-5]
Cryst. (EtOH). Mp 81°.

Marcuzzi, F. *et al*, *J.C.S. Perkin 1*, 1993, 2957 (*synth, pmr*)

2,4,5-Triphenyl-1,3,2,4,5-diselenatriphospholane T-1-00259

[132830-63-8]



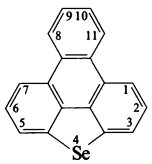
$C_{18}H_{15}P_3Se_2$ M 482.1

(***2α,4α,5β*)-form** [122039-28-5]
Yellow needles.

Wood, P.T. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1989, **41**, 51 (*synth, P-31 nmr, Se-77 nmr*)

Triphenyleno[1,12-*bcd*]selenophene T-1-00260

[149415-39-4]



$C_{18}H_{10}Se$ M 305.2
Cryst. Mp 184-185°.

Kimura, T. *et al*, *J.O.C.*, 1994, **59**, 7117 (*synth, pmr, cmr, Se-77 nmr*)

Triphenylmethanethiol, 9CI T-1-00261

α,α-Diphenylbenzenemethanethiol. Tritylthiol. Mercaptotriphenylmethane

[3695-77-0]

Ph_3CSH

$C_{19}H_{16}S$ M 276.4
Long prisms. Mp 107°.

S-*Ac:*
$C_{21}H_{18}OS$ M 318.4 Long needles (EtOH). Mp 139-141°.

S-*Me:*
$C_{20}H_{18}S$ M 290.4 Cryst. (MeOH). Mp 105-106°.

Disulfide: [15446-31-8]. *Bis(triphenylmethyl) disulfide. Ditrityl disulfide*
$C_{38}H_{30}S_2$ M 550.7 Yellow cryst. (hexane/CH_2Cl_2). Mp 156° dec.

Vorländer, D. *et al*, *Ber.*, 1913, **46**, 3450.
Ostrowski, M. *et al*, *Chem. Ber.*, 1993, **126**, 1355 (*disulfide, pmr, cmr, cryst struct*)

(Triphenylmethyl)phosphonothioic acid T-1-00262

Tritylthiophosphonic acid

$Ph_3CP(S)(OH)_2 \rightleftharpoons Ph_3CP(O)(OH)(SH)$

$C_{19}H_{17}O_2PS$ M 340.3
Tautomeric.

Thiophosphoryl-form

Difluoride: [149574-04-9].
$C_{19}H_{15}F_2PS$ M 344.3 Cryst. (CH_2Cl_2). Mp 192°.

Dichloride: [149574-03-8].
$C_{19}H_{15}Cl_2PS$ M 377.2 Cryst. (CH_2Cl_2). Mp 152°.

Goerlich, J.R. *et al*, *Z. Naturforsch., B*, 1993, **48**, 341 (*difluoride, dichloride, synth, ms, pmr, cmr*)

1,3,3-Triphenyl-1-propyne T-1-00263

1,1′,1″-(1-Propyl-1-yl-3-ylidene)trisbenzene, 9CI

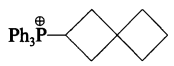
[5467-43-6]

$Ph_2CHC{\equiv}CPh$

$C_{21}H_{16}$ M 268.3
Prisms (petrol). Mp 79°.

Wieland, H. *et al*, *Annalen*, 1929, **470**, 201 (*synth*)
Chirko, A.I. *et al*, *Zh. Org. Khim.*, 1973, **9**, 1687; *J. Org. Chem. USSR (Engl. Transl.)*, 1709 (*synth, ir*)
Klett, M.W. *et al*, *J.A.C.S.*, 1985, **107**, 3963 (*pmr*)
Dem'yanov, P. *et al*, *Annalen*, 1995, 457 (*cmr*)

Triphenyl(spiro[3.3]hept-2-yl)phosphonium(1+) T-1-00264



$C_{25}H_{26}P^{\oplus}$ M 357.4 (ion)

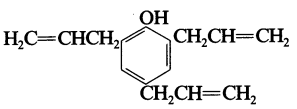
Bromide: [22997-61-1].
$C_{25}H_{26}BrP$ M 437.3 Cryst. (H_2O). Mp 188-190°.

Bestmann, H.J. *et al*, *Chem. Ber.*, 1969, **102**, 1802 (*synth*)

2,4,6-Tri-2-propenylphenol, 9CI T-1-00265

2,4,6-Triallylphenol

[20490-22-6]



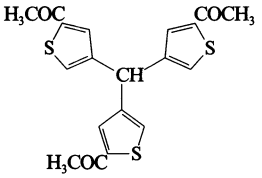
$C_{15}H_{18}O$ M 214.3
Liq. Bp 294°, Bp_1 116.2°.

Adv. Chem. Ser., 1955, **15**, 310 (***props***)
Davis, A.C. *et al*, *J.C.S.*, 1960, 888 (*synth*)
Mikhailov, B.M. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1968, 541; *CA*, **69**, 67448v (*synth*)
Crivello, J.V. *et al*, *Polym. Mater. Sci. Eng.*, 1992, **67**, 258 (*synth*)

Tris(5-acetyl-3-thienyl)methane T-1-00266

(1,1′,1″-Methylidynetri-4,2-thiophenediyl) trisethanone, 9CI

[43227-05-0]



$C_{19}H_{16}O_3S_3$ M 388.5
Forms host-guest inclusion compds.
Amorph. solid. Mp 50-58°.

Yakubov, A.P. *et al*, *J. Org. Chem. USSR (Engl. Transl.)*, 1973, **9**, 1549 (*synth*)
Din, L.B. *et al*, *Chem. Comm.*, 1977, **21**, 741 (*props*)
Pang, L. *et al*, *Acta Cryst. C*, 1994, **50**, 615 (*cryst struct, bibl*)

Tris(aminomethyl)phosphine T-1-00267

$P(CH_2NH_2)_3$

$C_3H_{12}N_3P$ M 121.1

Oxide: [17165-16-1].
$C_3H_{12}N_3OP$ M 137.1 Cryst. (EtOH) (as trihydrochloride). Mp 245-246° (trihydrochloride).

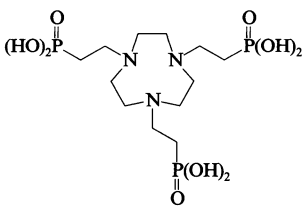
[71619-89-1]

Frank, A.W. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1981, **10**, 255.
Hägele, G. *et al*, *Z. Anorg. Allg. Chem.*, 1994, **620**, 914 (*derivs*)

1,4,6-Tris[2-(dihydroxyphosphinyl)ethyl]-1,4,7-triazacyclononane T-1-00268

[(Hexahydro-1H-1,4,7-triazonine-1,4,7-triyl) tri-2,1-ethanediyl]trisphosphonic acid, 9CI

[123325-12-2]



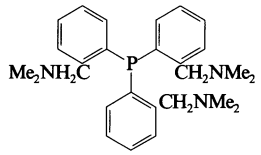
$C_{12}H_{30}N_3O_9P_3$ M 453.3
Complexing agent for Al(*III*), Fe(*III*), Ga(*III*), La(*III*) and rare earths. Cryst. (H_2O). Mp 264-266°. pK_{a1} <2; pK_{a2} 5.38; pK_{a3} 6.21; pK_{a4} 6.97; pK_{a5} 8.85; pK_{a6} 12.3.

Medved', T.Ya. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1988, 2103; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1988, 1886 (*synth, props, use*)
Pasechnik, M.P. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1992, 1776; *Bull. Russ. Acad. Sci., Div. Chem. Sci. (Engl. Transl.)*, 1992, 1377 (*complexes*)

Tris[2-(dimethylaminomethyl) phenyl]phosphine T-1-00269

2,2′,2″-Phosphinidynetris[N,N-*dimethylbenzenemethanamine*], *9CI*

[23936-58-5]



$C_{27}H_{36}N_3P$ M 433.5
Cryst. (EtOH/Et_2O). Mp 117-120°.

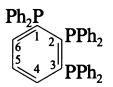
Monomethiodide: [152252-76-1]. *2-[Bis[2-(dimethylamino)methyl]phenyl]phosphino-*N,N,N-*trimethylbenzenemethanamium iodide, 9CI*
$C_{28}H_{39}IN_3P$ M 575.5 Powder (EtOH/C_6H_6). Mp 210-213°.

Chuit, C. *et al*, *Angew. Chem., Int. Ed.*, 1993, **32**, 1430 (*synth, ms, pmr, P-31 nmr, cryst struct*)

1,2,3-Tris(diphenylphosphino) benzene T-1-00270

1,2,3-Benzenetriyltris(diphenylphosphine), 9CI

[123739-94-6]



$C_{42}H_{33}P_3$ M 630.6
Solid. Mp 210-212°.

McFarlane, H.C.E. *et al*, *Polyhedron*, 1988, **7**, 1875 (*synth, P-31 nmr*)

1,2,4-Tris(diphenylphosphino) benzene T-1-00271

1,2,4-Benzenetriyltris(diphenylphosphine), 9CI

[123739-95-7]

$C_{42}H_{33}P_3$ M 630.6
Solid. Mp 142-144°.

McFarlane, H.C.E. *et al*, *Polyhedron*, 1988, **7**, 1875 (*synth, P-31 nmr*)

1,3,5-Tris(diphenylphosphino) benzene T-1-00272

1,3,5-Benzenetriyltris(diphenylphosphine), 9CI

[123739-96-8]

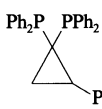
$C_{42}H_{33}P_3$ M 630.6
Solid. Mp 110-111°.

McFarlane, H.C.E. *et al*, *Polyhedron*, 1988, **7**, 1875 (*synth, P-31 nmr*)

1,1,2-Tris(diphenylphosphino) cyclopropane T-1-00273

1-Cyclopropyl-2-ylidenetris[diphenylphosphine], 9CI

[153477-75-9]



$C_{39}H_{33}P_3$ M 594.6
Triclinic cryst. (MeOH). Mp 139°.

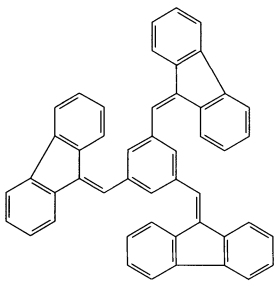
Borane complex (1:3): [153481-07-3]. [μ_3-[*1-Cyclopropanyl-2-ylidenetris[diphenylphosphine]*-P:P′:P″] *nonahydrotriboron], 9CI*
Cryst. ($CHCl_3$/pentane). Mp 180°.

Trioxide: [153477-76-0].
$C_{39}H_{33}O_3P_3$ M 642.6 Cryst. Mp 145°.

Trisulfide: [153477-77-1].
$C_{39}H_{33}P_3S_3$ M 690.8 Powder (THF/EtOH). Mp 223°.

Schmidtbaur, H. *et al*, *Chem. Ber.*, 1993, **126**, 2259 (*synth, ms, ir, pmr, cmr, P-31 nmr, cryst struct*)

1,3,5-Tris(9*H*-fluoren-9-ylidenemethyl)benzene T-1-00274



$C_{48}H_{30}$ M 606.7
Fine cryst. ($CHCl_3$/hexane). Mp 246-248°.

Mehta, G. *et al*, *J.C.S. Perkin 1*, 1995, 1787 (*synth, cryst struct, pmr, cmr*)

Tris(pentafluorophenyl) phosphite T-1-00275

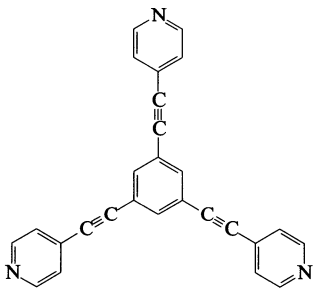
[86341-40-4]

$(C_6F_5O)_3P$

$C_{18}F_{15}O_3P$ M 580.1
Liq. or solid. Mp 39°. Bp_{10} 195°, $Bp_{0.05}$ 156-160°. n_D^{20} 1.4665.

Chauzov, V.A. *et al*, *Zh. Obshch. Khim.*, 1989, **59**, 1294 (*synth, P-31 nmr, reactions*)
Miranov, V.F. *et al*, *Zh. Obshch. Khim.*, 1991, **61**, 255; *J. Gen. Chem. USSR (Engl. Transl.)*, 1991, **61**, 232 (*synth, F-19 nmr, P-31 nmr*)

1,3,5-Tris(4-pyridylethynyl) benzene T-1-00276



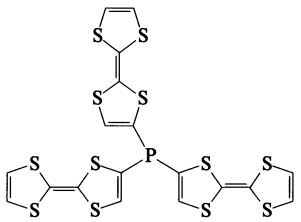
$C_{27}H_{15}N_3$ M 381.4
Yellow-orange solid. Mp >200° dec.

Anderson, H.L. *et al*, *J.C.S. Perkin 1*, 1995, 2275 (*synth, ir, pmr*)

Tris(tetrathiafulvalenyl) phosphine T-1-00277

Tris[2-(1,3-dithiol-2-yldiene)-1,3-dithiol-4-yl] phosphine

[137552-55-7]



$C_{18}H_9PS_{12}$ M 641.0
Solid.

Fourmigue, M. *et al*, *Chem. Comm.*, 1991, 1370 (*synth, P-31 nmr, cryst struct*)

1,2,3-Tris(trifluoromethyl) benzene, 9CI T-1-00278

[42175-48-4]

$C_9H_3F_9$ M 282.1

Lukmanov, V.G. *et al*, *Zh. Org. Khim.*, 1973, **9**, 1019; *CA*, **79**, 42101v (*synth*)

1,2,4-Tris(trifluoromethyl) benzene, 9CI T-1-00279

[393-05-5]

$C_9H_3F_9$ M 282.1
Bp_{100} 79-80°. n_D^{25} 1.3679.

Krespan, C.G. *et al*, *J.A.C.S.*, 1961, **83**, 3428 (*synth*)

1,3,5-Tris(trifluoromethyl) benzene, 9CI T-1-00280

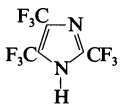
α,α,α,α′,α′,α′,α″,α″,α″-*Nonafluoromesitylene*

[729-81-7]

$C_9H_3F_9$ M 282.1
d 1.51. Mp 9°. Bp 118-119°. n_D^{25} 1.3558.

McBee, E.T. *et al*, *Ind. Eng. Chem.*, 1947, **39**, 393 (*synth*)
Cooper, C.D. *et al*, *J. Chem. Phys.*, 1952, **20**, 1903 (*uv*)

2,4,5-Tris(trifluoromethyl) imidazole T-1-00281

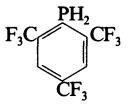


$C_6HF_9N_2$ M 272.0
Cryst. by subl. Mp 139-141°.

Owen, D. *et al*, *J. Fluorine Chem.*, 1981, **17**, 179 (*synth, pmr, F-19 nmr*)

[2,4,6-Tris(trifluoromethyl)phenyl]phosphine, 9CI T-1-00282

[124927-09-9]

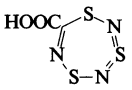


$C_9H_4F_9P$ M 314.0
Air-sensitive liq. Bp_{12} 56-58°.

Scholz, M. *et al*, *J. Organomet. Chem.*, 1989, **366**, 73 (*synth, pmr, F-19 nmr, P-31 nmr*)

$3\delta^2,3\lambda^4$-1,3,5,2,4,6-Trithiatriazepine-7-carboxylic acid, 9CI T-1-00283

[116509-19-4]



$C_2HN_3O_2S_3$ M 195.2
Needles (H_2O). Mp 149-150° dec.

Me ester: [89929-35-1].
$C_3H_3N_3O_2S_3$ M 209.2 Synth. from S_4N_4 + MeOOCC≡CCOOMe. Cryst. (petrol). Mp 81-83°.

tert-*Butyl ester:* [109988-32-1].
$C_6H_9N_3O_2S_3$ M 251.3 Needles (petrol). Mp 82.5-83°.

Azide: [124613-13-4].
$C_2N_6OS_3$ M 220.2 Needles (petrol). Mp 75-76°.

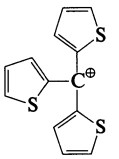
Amide: [124613-18-9].
$C_2H_2N_4OS_3$ M 194.2 Cryst. ($EtOAc/CH_2Cl_2$). Mp 180°.

Anhydride: [124635-36-5].
$C_4N_6O_3S_6$ M 372.4 Cryst. Mp 120-125°.

Daley, S.T.A.K. *et al*, *Chem. Comm.*, 1984, 55 (*cryst struct, Me ester*)
Daley, S.T.A.K. *et al*, *J.C.S. Perkin 1*, 1987, 203 (*synth, ir, uv, pmr, Me ester*)
Dunn, P.J. *et al*, *J.C.S. Perkin 1*, 1988, 1745; 1989, 1405 (*synth, uv, ir, pmr, ms*)

Tri-2-thienylmethylium(1+), 9CI T-1-00284

Tris(2-thienyl)methyl



$C_{13}H_9S_3^{\oplus}$ M 261.4 (ion)

Perchlorate: [112401-10-2].
$C_{13}H_9ClO_4S_3$ M 360.8 Brown cryst. Racemic mixt. of 2 enantiomeric conforms.

Abarca, B. *et al*, *J.O.C.*, 1991, **56**, 3224 (*synth*)
Varea, T. *et al*, *Chem. Comm.*, 1993, 1476 (*synth, cryst struct*)

1,2,3-Trithiolane, 9CI T-1-00285

1,2,3-Trithiacyclopentane

$C_2H_4S_3$ M 124.2

2-Oxide: [153898-66-9].
$C_2H_4OS_3$ M 140.2 Pale yellow oil.

Yomoji, N. *et al*, *J.C.S. Perkin 1*, 1993, 1995 (*oxide, synth, ir, uv, pmr, cmr*)

U

3,9-Undecadiyn-1-ol **U-1-00001**

[92013-73-5]

$H_3CC{\equiv}C(CH_2)_4C{\equiv}CCH_2CH_2OH$

$C_{11}H_{16}O$ M 164.2
Oil.

Bao, J. *et al*, *J.A.C.S.*, 1994, **116**, 7616 (*synth, ir, pmr, cmr, ms*)

4,9-Undecadiyn-1-ol **U-1-00002**

[160109-65-9]

$H_3CC{\equiv}C(CH_2)_3C{\equiv}CCH_2CH_2CH_2OH$

$C_{11}H_{16}O$ M 164.2
No phys. props. descr.

Bao, J. *et al*, *J.A.C.S.*, 1994, **116**, 7616 (*synth, ir, pmr, cmr, ms*)

1-Undecen-5-one, 9CI **U-1-00003**

[38945-65-2]

$H_3C(CH_2)_5COCH_2CH_2CH{=}CH_2$

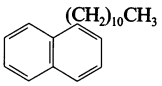
$C_{11}H_{20}O$ M 168.2
Liq. Bp 225-226°, $Bp_{0.2}$ 61-64°. n_D^{20} 1.4388.

Naoshima, Y. *et al*, *Agric. Biol. Chem.*, 1979, **43**, 1765 (*synth, ir, pmr*)
Ho, T.-L., *Synth. Commun.*, 1981, **11**, 7 (*synth, ir, pmr*)
Vermeer, P. *et al*, *J. Organomet. Chem.*, 1986, **301**, 247 (*synth, ir, pmr*)
Ballini, R. *et al*, *Synthesis*, 1994, 723 (*synth, pmr*)

1-Undecylnaphthalene **U-1-00004**

1-(1-Naphthalenyl)undecane

[7225-71-0]



$C_{21}H_{30}$ M 282.4
d^{20} 0.928. Fp 23°. Bp 401°, Bp_2 177°. n_D^{20} 1.5399.

Adv. Chem. Ser., 1955, **15**, 234 (***props***)

2-Undecylnaphthalene **U-1-00005**

1-(2-Naphthalenyl)undecane

$C_{21}H_{30}$ M 282.4
d^{20} 0.921. Fp 20°. Bp 401°, Bp_1 177°. n_D^{20} 1.5376.

Adv. Chem. Ser., 1955, **15**, 235 (***props***)

6-Undecyn-5-one, 9CI **U-1-00006**

[30611-17-7]

$H_3C(CH_2)_3C{\equiv}CCO(CH_2)_3CH_3$

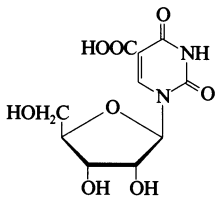
$C_{11}H_{18}O$ M 166.2
Liq. Bp_{15} 112-113°. n_D^{20} 1.4510.

Bourgain, M. *et al*, *Bull. Soc. Chim. Fr.*, 1973, 2137 (*synth, ir, pmr*)
Cahiez, G. *et al*, *Synthesis*, 1977, 130 (*synth*)
Gleiter, R. *et al*, *Synthesis*, 1995, 969 (*synth, pmr, cmr, ir*)

5-Uridinecarboxylic acid **U-1-00007**

1,2,3,4-Tetrahydro-2,4-dioxo-1-β-D-ribofuranosyl-5-pyrimidinecarboxylic acid, 9CI

[3180-22-1]



$C_{10}H_{12}N_2O_8$ M 288.2
Needles (EtOH aq.). Mp 118°. pK_a 9.5, 4.2.

Amide: [110914-06-2].
$C_{10}H_{13}N_3O_7$ M 287.2 Needles (EtOH). Mp 198-200° dec.

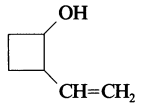
Nitrile: [4425-57-4]. *5-Cyanouridine,* 9CI
$C_{10}H_{11}N_3O_6$ M 269.2 Needles (EtOH). Mp 185°. $[\alpha]_D^{25}$ −4.7.

Imai, K. *et al*, *Chem. Pharm. Bull.*, 1965, **13**, 7 (*synth, uv*)
Cusack, N.J. *et al*, *J.C.S. Perkin 1*, 1973, 1720 (*nitrile*)
Agathocleous, D.C. *et al*, *J.C.S. Perkin 1*, 1991, 2317 (*amide, pmr*)

V

2-Vinylcyclobutanol V-1-00001

2-Ethenylcyclobutanol



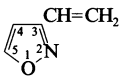
$C_6H_{10}O$ M 98.1

cis- and *trans*-isomers prepd. and sepd. by glc.

Harris, N.J. *et al*, *J.A.C.S.*, 1994, **116**, 6121 (*synth, ir, pmr, cmr*)

3-Vinylisoxazole V-1-00002

3-Ethenylisoxazole



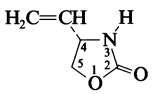
C_5H_5NO M 95.1

Pale yellow oil.

Ambler, P.W. *et al*, *Chem. Comm.*, 1994, 2661 (*synth, pmr*)

4-Vinyl-2-oxazolidinone V-1-00003

4-Ethenyl-2-oxazolidinone, 9CI



$C_5H_7NO_2$ M 113.1

(*S*)-*form* [146565-74-4]

Pale yellow oil. $[\alpha]_D^{20}$ −17.6 (c, 1.0 in $CHCl_3$).

Yoo, S. *et al*, *J.O.C.*, 1994, **59**, 6968 (*synth, pmr, cmr, ms*)

Vinylphosphonous diamide, V-1-00004

8CI

Ethenylphosphonous diamide, 9CI

$H_2C{=}CHP(NH_2)_2$

$C_2H_7N_2P$ M 90.0

N,N,N′,N′-*Tetra-Me:* [53422-58-5]. P-*Ethenyl*-N,N,N′,N′-*tetramethylphosphonous diamide. Vinylphosphonous bis(dimethylamide)*

$C_6H_{15}N_2P$ M 146.1 Liq. Bp_{28} 75-79°.

N,N,N′,N′-*Tetra-Et:* [89438-02-8]. P-*Ethenyl*-N,N,N′,N′-*tetraethylphosphonous amide. Vinylphosphonous bis(diethylamide)*

$C_{10}H_{23}N_2P$ M 202.2 Liq. $Bp_{1.4\text{-}1.6}$ 65-70°, $Bp_{0.02}$ 45-46°.

N,N,N′,N′-*Tetraisopropyl:* [89438-04-0]. *Vinylphosphonous bis(diisopropylamide)*. P-*Ethenyl*-N,N,N′,N′-*tetrakis(1-methylethyl) phosphonous diamide*

$C_{14}H_{31}N_2P$ M 258.3 Solid. Mp 26-27°. $Bp_{0.3}$ 77-80°.

N,N,N′,N′-*Tetrakis(trimethylsilyl):* [122631-80-5]. P-*Ethenyl*-N,N,N′,N′-*tetrakis(trimethylsilyl)phosphonous diamide*

$C_{14}H_{39}N_2PSi_4$ M 378.7 Liq. $Bp_{0.01}$ 61-65°.

King, R.B. *et al*, *J.A.C.S.*, 1977, **99**, 4001 (*tetra-Me, synth, cmr, P-31 nmr*)

King, R.B. *et al*, *J.O.C.*, 1984, **49**, 1784 (*synth, ms, pmr, cmr, P-31 nmr*)

Vierling, P. *et al*, *Organometallics*, 1986, **5**, 2543 (*tetra-Et, synth, ir, pmr, P-31 nmr*)

Waters, K.E. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1988, **39**, 189 (*synth, cmr, P-31 nmr*)

Fluck, E. *et al*, *Z. Anorg. Allg. Chem.*, 1992, **613**, 31 (*tetra-Et, synth, ir, P-31 nmr*)

Vinylphosphonous dibromide, V-1-00005

8CI

Ethenylphosphonous dibromide, 9CI. Dibromovinylphosphine

[41813-13-2]

$H_2C{=}CHPBr_2$

$C_2H_3Br_2P$ M 217.8

Pale yellow fuming liq. d_4^{20} 2.27. Bp_{20} 60°. n_D^{20} 1.6915.

Bartocha, B. *et al*, *Z. Naturforsch., B*, 1959, **14**, 809 (*synth*)

Levin, Ya.A. *et al*, *Zh. Obshch. Khim.*, 1973, **43**, 283; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1973, **43**, 282 (*synth*)

Althoff, A. *et al*, *Chem. Ber.*, 1978, **111**, 1845 (*synth, P-31 nmr*)

Diemert, K. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1986, **26**, 307 (*synth, P-31 nmr*)

Vinylphosphonous dichloride, V-1-00006

8CI

Ethenylphosphonous dichloride, 9CI. Dichlorovinylphosphine

[3541-56-8]

$H_2C{=}CHPCl_2$

$C_2H_3Cl_2P$ M 128.9

Liq. which fumes in air. Sensitive to air and moisture. d^{20} 1.30. Bp 105°, Bp_{200} 63-65°. n_D^{20} 1.5145.

Kaesz, H.D. *et al*, *J.O.C.*, 1959, **24**, 635 (*synth, ir*)

Levin, Ya.A. *et al*, *Zh. Obshch. Khim.*, 1973, **43**, 281; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1973, **43**, 280 (*synth*)

Naumov, V.A. *et al*, *Zh. Strukt. Khim.*, 1984, **25**, 137.

Diemert, K. *et al*, *Phosphorus Sulfur Relat. Elem.*, 1986, **26**, 307 (*synth, P-31 nmr*)

Zverev, V.V. *et al*, *Metalloorg. Khim.*, 1990, **3**, 1012; *Organometallic Chem. USSR* (*Engl. Transl.*), 1990, **3**, 516 (*pe, theory*)

Ermolaeva, L.V. *et al*, *Metalloorg. Khim.*, 1990, **3**, 1156; *Organometallic Chem. USSR* (*Engl. Transl.*), 1990, **3**, 598 (*conformn, theory*)

Zverev, V.V. *et al*, *Zh. Strukt. Khim.*, 1990, **31**, 65; *J. Struct. Chem.* (*Engl. Transl.*), 1990, **31**, 904 (*pe, theory*)

Chernova, A.V. *et al*, *Zh. Obshch. Khim.*, 1993, **63**, 2603; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1993, **63**, 1807 (*ir, Raman*)

4-Vinylpiperidine V-1-00007

4-Ethenylpiperidine

[7613-15-2]

$C_7H_{13}N$ M 111.1

$Bp_{14.5}$ 134-135°.

N-*Ac:*

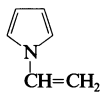
$C_9H_{15}NO$ M 153.2 $Bp_{13.5}$ 133°.

Perry, R.A. *et al*, *Can. J. Chem.*, 1976, **54**, 2385 (*synth, ir, pmr*)

1-Vinyl-1*H*-pyrrole V-1-00008

1-Ethenyl-1H-pyrrole, 9CI

[13401-81-5]



C_6H_7N M 93.1

Liq. Bp 122°, Bp_{15} 28°. n_D^{20} 1.5260.

Reppe, W. *et al*, *Annalen*, 1956, **601**, 81 (*synth*)

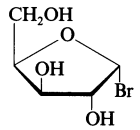
Sigalov, M.V. *et al*, *Tetrahedron*, 1981, **37**, 3051 (*cmr, pmr*)

Attaryan, O.S. *et al*, *Zh. Org. Khim.*, 1988, **24**, 1339; *J. Org. Chem. USSR* (*Engl. Transl.*), 1988, **24**, 1206 (*synth, ir, pmr*)

Trofimov, B.A. *et al*, *Synth. Commun.*, 1994, **24**, 2035 (*synth, pmr*)

X

Xylofuranosyl bromide X-1-00001



α-D-*form*

$C_5H_9BrO_4$ M 213.0

α-D-form

Tri-Ac: [55057-30-2].
$C_{11}H_{15}BrO_7$ M 339.1 Syrup.

Tribenzoyl: [38837-18-2].
$C_{26}H_{21}BrO_7$ M 525.3 Syrup.

β-D-form

Tri-Ac: [55057-31-3].
Syrup.

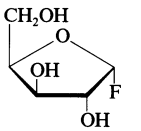
Tribenzoyl: [38837-19-3].
Syrup.

Wagner, G. *et al*, *Pharmazie*, 1972, **27**, 433 (*α-tribenzoyl, β-tribenzoyl*)

Bock, K. *et al*, *Acta Chem. Scand., Ser. B*, 1974, **28**, 1041; 1975, **29**, 185 (*α-tri-Ac, β-tri-Ac, pmr*)

Girodeau, J.M. *et al*, *J. Antibiot.*, 1984, **37**, 150 (*deriv*)

Xylofuranosyl fluoride X-1-00002



α-D-*form*

$C_5H_9FO_4$ M 152.1

α-D-form

2-Me, 3,5-dibenzoyl: [38791-48-9].
$C_{20}H_{19}FO_6$ M 374.3 Syrup. $[\alpha]_D^{25}$ −32.5 (c, 0.65 in $CHCl_3$).

β-D-form

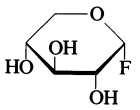
Tri-Ac: [28072-59-5].
$C_{11}H_{15}FO_7$ M 278.2 Syrup.

2-Me, 3,5-dibenzoyl: [38791-49-0].
Cryst. (Et_2O/pentane). Mp 82-83°. $[\alpha]_D^{22}$ −133 (c, 1.6 in $CHCl_3$).

Hall, L.D. *et al*, *Can. J. Chem.*, 1970, **48**, 1155 (*tri-Ac, pmr, F-19 nmr*)

Jacobsen, S. *et al*, *Acta Chem. Scand.*, 1972, **26**, 1561 (*deriv, pmr, F-19 nmr*)

Xylopyranosyl fluoride X-1-00003



α-D-*form*

$C_5H_9FO_4$ M 152.1

α-D-form [4536-02-1]

Tri-Ac: [440-05-1].
$C_{11}H_{15}FO_7$ M 278.2 Cryst. Mp 86-88°. $[\alpha]_D$ +67.2 (c, 1.0 in $CHCl_3$).

Tribenzoyl: [4163-50-2].
$C_{26}H_{21}FO_7$ M 464.4 Needles (EtOH or Et_2O/pentane). Mp 119-120°. $[\alpha]_D^{20}$ +39.2 (c, 0.93 in $CHCl_3$).

2-Me, 3,4-dibenzoyl: [38791-46-7].
$C_{20}H_{19}FO_6$ M 374.3 Cryst. (Et_2O/pentane). Mp 120-121°. $[\alpha]_D^{23}$ −56.7 (c, 0.3 in $CHCl_3$).

Tribenzyl: [95898-05-8].
$C_{26}H_{27}FO_4$ M 422.4 Syrup.

β-D-form [108393-17-5]

Tri-Ac: [10369-21-8].
Mp 56-57° (52-55°). $[\alpha]_D^{23}$ −56.4 (c, 1.6 in $CHCl_3$).

Tribenzoyl: [3862-87-1].
Prisms (EtOH). Mp 149-150°. $[\alpha]_D^{20}$ −39.4 (c, 1.04 in $CHCl_3$).

2-Me, 3,4-dibenzoyl: [38791-47-8].
Cryst. (Et_2O/pentane). Mp 82-83°. $[\alpha]_D^{22}$ −133 (c, 1.6 in $CHCl_3$).

Brauns, D.K., *J.A.C.S.*, 1923, **45**, 833 (*α-tri-Ac*)

Pedersen, C., *Acta Chem. Scand.*, 1963, **17**, 1269 (*tribenzoyl*)

Lundt, K. *et al*, *Mikrochim. Acta*, 1966, 126 (*β-tri-Ac*)

Hall, L.D. *et al*, *Carbohydr. Res.*, 1967, **4**, 512; 1969, **9**, 11 (*pmr*)

Hall, L.D. *et al*, *Can. J. Chem.*, 1969, **47**, 19 (*tri-Ac, pmr, F-19 nmr*)

Jacobsen, S. *et al*, *Acta Chem. Scand.*, 1972, **26**, 1561 (*α-Me deriv, β-Me deriv, pmr*)

Kasumi, T. *et al*, *Biochemistry*, 1987, **26**, 3010 (*pmr, F-19 nmr*)

Yamada, H. *et al*, *Tet. Lett.*, 1987, **28**, 4315 (*tribenzyl*)

Name Index

The Name Index lists in alphabetical order all names and synonyms contained in the Dictionary.

Each index term refers the user to a Dictionary Number consisting of a single letter of the alphabet followed by six digits. The letter is the first letter of the relevant Entry Name. The first digit of the Dictionary Number refers to the number of the Supplement in which the Entry appears. In this, the First Supplement, the first digit is invariably 1.

A Dictionary Number which follows immediately upon an index term means that the term is itself used as the Entry Name.

A Dictionary Number which is preceded by the word '*see*' means that the term is a synonym to an Entry Name.

A Dictionary Number which is preceded by the word '*in*' means that the term is embedded within an Entry, usually as a synonym to a particular stereoisomeric form or to a derivative,

The symbol ▶ preceding an index term indicates that the Dictionary Entry contains information on toxic or hazardous properties of the compound.

The symbol † following an index term indicates that the name is known to the editors as being a duplicate and has been assigned to two or more different compounds.

Name Index

Molecular Formula Index

The Molecular Formula Index lists the molecular formula of all compounds in the Dictionary whether they occur as main Entry compounds or as derivatives.

The first digit of the Dictionary Number refers to the number of the Supplement in which the Entry appears. In this, the First Supplement, the first digit is invariably 1.

Where a molecular formula applies to a compound listed as a derivative the Dictionary Number is prefixed by the word '*in*'.

The symbol ▶ preceding an index term indicates that the Dictionary Entry contains information on toxic or hazardous properties of the compound.

The symbol † refers to a name which is known to be a duplicated name.

Molecular Formula Index

5-(Hydroxymethyl)-3-pyridinecarboxylic acid; Et ester, *in* H-1-00138
6-(Hydroxymethyl)-2-pyridinecarboxylic acid; Et ester, *in* H-1-00139
6-(Hydroxymethyl)-3-pyridinecarboxylic acid; Et ester, *in* H-1-00140

$C_9H_{11}NO_7$
2-β-D-Ribofuranosyl-4-oxazolecarboxylic acid, R-1-00003

$C_9H_{11}NS$
2-Phenylthiazolidine, P-1-00104
4-Phenylthiazolidine, P-1-00105
5-Phenylthiazolidine, P-1-00106

$C_9H_{11}N_2O_8P$
Cyclic UMP, C-1-00187

$C_9H_{11}N_5O_4$
2′-Azido-2′,3′-dideoxyuridine, A-1-00254

$C_9H_{11}P$
1-Phenylphosphetane, P-1-00091

$C_9H_{12}ClN$
1-(4-Chlorophenyl)-2-propylamine, C-1-00156

$C_9H_{12}ClN_3O_3$
5-Chloro-2′,3′-dideoxycytidine, C-1-00071

$C_9H_{12}ClO_3P$
Dimethyl (α-chlorobenzyl)phosphonate, *in* C-1-00024

$C_9H_{12}Cl_2O_8S$
5-Chloro-5-deoxyxylose; 1,2-Di-Ac, 3-chlorosulfate, *in* C-1-00062

$C_9H_{12}FN_3O_3$
2′,3′-Dideoxy-2′-fluorocytidine, D-1-00215
F-DDC, *in* D-1-00215

$C_9H_{12}FN_3O_4$
2′-Deoxy-2′-fluorocytidine, D-1-00019

$C_9H_{12}F_2O_5$
2-Deoxy-2-fluoroarabinopyranosyl fluoride; Di-Ac, *in* D-1-00017
2-Deoxy-2-fluorolyxopyranosyl fluoride; Di-Ac, *in* D-1-00031
2-Deoxy-2-fluororibopyranosyl fluoride; Di-Ac, *in* D-1-00035
2-Deoxy-2-fluoroxylopyranosyl fluoride; Di-Ac, *in* D-1-00039
3-Deoxy-3-fluoroxylopyranosyl fluoride; Di-Ac, *in* D-1-00040

$C_9H_{12}N_2$
3-Amino-3-phenylazetidine, A-1-00191
1,2-Dicyanocycloheptane, *in* C-1-00192

$C_9H_{12}N_2O$
N,N′-Dimethyl-*N*-phenylurea, D-1-00464

$C_9H_{12}N_2O_2$
3-Nitro-2-phenyl-1-propylamine, N-1-00031

$C_9H_{12}N_2O_4$
2′,3′-Dideoxyuridine, D-1-00220

$C_9H_{12}N_2O_4S$
2′-Deoxy-4′-thiouridine, D-1-00078

$C_9H_{12}N_2O_5$
2′-Deoxypseudouridine, D-1-00075

$C_9H_{12}N_2O_6$
2-β-D-Ribofuranosyl-4-oxazolecarboxamide, *in* R-1-00003

$C_9H_{12}N_3O_7P$
Cyclic CMP, C-1-00185

$C_9H_{12}N_4O_4$
2-Amino-3,5-dinitropyridine; *N,N*-Di-Et, *in* A-1-00130

$C_9H_{12}O$
Bicyclo[6.1.0]non-1(8)-en-9-one, B-1-00095
2-Cyclononyn-1-one, C-1-00210
1,3,3*a*,4,7,7*a*-Hexahydro-2*H*-inden-2-one, H-1-00042
1,2,3,6,7,7*a*-Hexahydro-5*H*-inden-5-one, H-1-00043
3,7-Nonadiyn-1-ol, N-1-00042

$C_9H_{12}O_2$
Bicyclo[5.1.1]nonane-3,5-dione, B-1-00093

$C_9H_{12}O_3$
3-Acetylbicyclo[1.1.1]pentane-1-carboxylic acid; Me ester, *in* A-1-00012
Hexahydro-1*H*-cyclohepta[*c*]furan-1,3-(3*aH*)-dione, *in* C-1-00192
2-(Phenoxymethoxy)ethanol, *in* H-1-00103

$C_9H_{12}O_4$
Bicyclo[4.1.0]heptane-7,7-dicarboxylic acid, B-1-00083
1,2-Spiropentanedicarboxylic acid; Di-Me ester, *in* S-1-00005

$C_9H_{12}O_6$
Gabosine G, *in* T-1-00227

$C_9H_{12}S$
2-Isopropylbenzenethiol, I-1-00072
4-Isopropylbenzenethiol, I-1-00073
Isopropyl phenyl sulfide, I-1-00082
1-Methyl-2[(methylthio)methyl]benzene, *in* M-1-00024
1-Methyl-4[(methylthio)methyl]benzene, *in* M-1-00026

$C_9H_{12}S_2$
Benzyl ethyl disulfide, B-1-00067

$C_9H_{13}Br$
3-Bromotricyclo[3.3.1.0^{3,7}]nonane, B-1-00400

$C_9H_{13}BrN_2O_2$
▶ Pyridostigmine bromide, *in* P-1-00178

$C_9H_{13}Cl$
3-Chlorotricyclo[3.3.1.0^{3,7}]nonane, C-1-00170

$C_9H_{13}ClO$
3-Cyclohexyl-2-propenoic acid; Chloride, *in* C-1-00207

$C_9H_{13}ClO_6$
2-Chloro-2-deoxyxylose; 3,4-Di-Ac, *in* C-1-00059

$C_9H_{13}IO_4$
3,6-Anhydro-5-deoxy-5-iodoidofuranose; 1,2-*O*-Isopropylidene, *in* A-1-00233

$C_9H_{13}N$
9-Azabicyclo[3.3.1]nona-2,6-diene; *N*-Me, *in* A-1-00240
1-Cyano-2-cyclohexylethylene, *in* C-1-00207

$C_9H_{13}NO$
1-Aminobicyclo[2.2.1]hept-2-ene; *N*-Ac, *in* A-1-00063
5-Aminobicyclo[2.2.1]hept-2-ene; *N*-Ac, *in* A-1-00064
1-(3-Aminophenyl)ethanol; *N*-Me, *in* A-1-00193
3-Amino-1-phenyl-1-propanol, A-1-00199

$C_9H_{13}NO_2$
(1-Ethylpropylidene)propanedioic acid; Mononitrile, Me ester, *in* E-1-00025

$C_9H_{13}NO_2S$
2-(4-Methylbenzenesulfonyl)ethylamine, M-1-00027

$C_9H_{13}N_2O_2^{\oplus}$
▶ Pyridostigmine(1+), P-1-00178

$C_9H_{13}N_3O_3S$
2′-Deoxy-4′-thiocytidine, D-1-00077

$C_9H_{13}O_3P$
(2-Isopropylphenyl)phosphonic acid, I-1-00080
(4-Isopropylphenyl)phosphonic acid, I-1-00081

$C_9H_{14}NO_2P$
(3-Aminopropyl)phenylphosphinic acid, A-1-00202

$C_9H_{14}N_2O_4$
α-Amino-2,3-dihydro-5-methyl-3-oxo-4-isoxazolepropanoic acid; Et ester, *in* A-1-00119

$C_9H_{14}O$
Bicyclo[5.1.1]nonan-4-one, B-1-00094
3,5-Dimethyl-3-cyclohexene-1-carboxaldehyde, D-1-00386
2,4-Dimethyl-2,4-heptadienal, D-1-00404

$C_9H_{14}O_2$
3-Cyclohexene-1-acetic acid; Me ester, *in* C-1-00197
3-Cyclohexyl-2-propenoic acid, C-1-00207
8-Nonene-2,5-dione, N-1-00048
4*H*,6*H*-3*a*,6*a*-Propano-1*H*,3*H*-furo[3,4-*c*]furan, P-1-00130

$C_9H_{14}O_3$
2-Hydroxycycloheptanone; Ac, *in* H-1-00072
2-Oxocyclopentaneacetic acid; Et ester, *in* O-1-00040

$C_9H_{14}O_4$
1,2-Cycloheptanedicarboxylic acid, C-1-00192

$C_9H_{14}O_5$
3-Oxoheptanedioic acid; Di-Me ester, *in* O-1-00045

$C_9H_{14}O_6$
1,1,1-Ethanetricarboxylic acid; Et, Di-Me ester, *in* E-1-00009

$C_9H_{15}Br$
1-Bromo-3-*tert*-butylbicyclo[1.1.1]pentane, B-1-00235

$C_9H_{15}BrO_4$
5-Bromo-5-deoxyribose; Me glycoside, 2,3-*O*-isopropylidene, *in* B-1-00265
5-Bromo-5-deoxyxylose; 1,2-*O*-Isopropylidene, 3-Me, *in* B-1-00273

$C_9H_{15}BrO_5$
5-Bromo-5-deoxyidose; 1,2-*O*-Isopropylidene, *in* B-1-00255
6-Bromo-6-deoxysorbose; 2,3-*O*-Isopropylidene, *in* B-1-00266

$C_9H_{15}ClO_2$
2,3-Dimethylcyclopentanol; Chloroacetate, *in* D-1-00389

$C_9H_{15}ClO_4$
5-Chloro-5-deoxyribose; Me glycoside, 2,3-*O*-isopropylidene, *in* C-1-00055

$C_9H_{15}ClO_5$
1-Chloro-1-deoxyfructose; 2,3-*O*-Isopropylidene, *in* C-1-00042
6-Chloro-6-deoxyfructose; 2,3-*O*-Isopropylidene, *in* C-1-00044
5-Chloro-5-deoxyidose; 1,2-*O*-Isopropylidene, *in* C-1-00048
6-Chloro-6-deoxyidose; 1,2-*O*-Isopropylidene, *in* C-1-00049
1-Chloro-1-deoxysorbose; 2,3-*O*-Isopropylidene, *in* C-1-00056
6-Chloro-6-deoxytalose; 1,2-*O*-Isopropylidene, *in* C-1-00058

$C_9H_{15}ClO_6S$
5-Chloro-5-deoxyarabinose; 1,2-*O*-Isopropylidene, 3-mesyl, *in* C-1-00041
5-Chloro-5-deoxyxylose; 1,2-*O*-Isopropylidene, 3-mesyl, *in* C-1-00062

$C_9H_{15}FO_5$
3-Deoxy-3-fluoroidose; 1,2-*O*-Isopropylidene, *in* D-1-00030

$C_9H_{15}IO_4$
5-Deoxy-5-iodolyxose; Me glycoside, 2,3-*O*-isopropylidene, *in* D-1-00059
5-Deoxy-5-iodoribose; Me glycoside, 2,3-*O*-isopropylidene, *in* D-1-00066

$C_9H_{15}IO_5$
3-Deoxy-3-iodoallose; 1,2-*O*-Isopropylidene, *in* D-1-00043
1-Deoxy-1-iodosorbose; 2,3-*O*-Isopropylidene, *in* D-1-00067
3-Deoxy-3-iodoxylose; Me glycoside, 4-Me, 2-Ac, *in* D-1-00072

$C_9H_{15}N$
5-Aminobicyclo[2.2.1]hept-2-ene; *N,N*-Di-Me, *in* A-1-00064

4-Methyl-5-benzofurancarboxaldehyde, M-1-00031
5-Methyl-2-benzofurancarboxaldehyde, M-1-00032
5-Methyl-3-benzofurancarboxaldehyde, M-1-00033
6-Methyl-2-benzofurancarboxaldehyde, M-1-00034
6-Methyl-3-benzofurancarboxaldehyde, M-1-00035
7-Methyl-2-benzofurancarboxaldehyde, M-1-00036

$C_{10}H_8O_2S$
3-(Methylthio)-4*H*-1-benzopyran-4-one, *in* M-1-00007

$C_{10}H_8O_2S_6$
2,2′-Bi(5,6-dihydro-1,3-dithiolo[4,5-*b*][1,4]oxathiin-2-ylidene), B-1-00102

$C_{10}H_8O_3$
5-Acetyl-4-hydroxybenzofuran, A-1-00030
6-Methoxy-5-benzofurancarboxaldehyde, *in* H-1-00061
1-Oxo-2-indanecarboxylic acid, O-1-00046

$C_{10}H_8O_4$
3,8-Dioxatricyclo[5.3.1.1^{2,6}]dodeca-4,9-diene-11,12-dione, D-1-00491

$C_{10}H_9BrN_2O$
6-Bromo-1*H*-indole-3-acetamide, *in* B-1-00304

$C_{10}H_9ClO_4$
2-(Chloroacetoxymethyl)benzoic acid, C-1-00011

$C_{10}H_9Cl_2NO$
5,6-Dichloro-3,4-dihydro-1(2*H*)-naphthalenone; Oxime, *in* D-1-00176
6,7-Dichloro-3,4-dihydro-1(2*H*)-naphthalenone; Oxime, *in* D-1-00177

$C_{10}H_9FO_3$
4-(4-Fluorophenyl)-4-oxobutanoic acid, F-1-00052

$C_{10}H_9F_3O_2$
3-(Trifluoromethyl)benzeneacetic acid; Me ester, *in* T-1-00191

$C_{10}H_9N$
1*H*-1-Benzazepine, B-1-00001
3*H*-2-Benzazepine, B-1-00002

$C_{10}H_9NO$
3-Oxiranyl-1*H*-indole, O-1-00038

$C_{10}H_9NO_2$
4-(4-Hydroxyphenyl)-4-oxobutanenitrile, *in* H-1-00171
2-Indolizinecarboxylic acid; Me ester, *in* I-1-00016
3-Indolizinecarboxylic acid; Me ester, *in* I-1-00017
Isocyanoacetic acid; Benzyl ester, *in* I-1-00067
2-Methyl-4-phenyl-5(2*H*)-isoxazolone, *in* H-1-00170
3-Phenyl-2,5-pyrrolidinedione, P-1-00096

$C_{10}H_9NO_2S$
2,3-Dihydro-2-thioxo-1*H*-indole-3-acetic acid, D-1-00332

$C_{10}H_9NO_3$
1-Oxo-2-indanecarboxylic acid; Oxime, *in* O-1-00046

$C_{10}H_9N_2P$
Bis(cyanomethyl)phenylphosphine, *in* P-1-00092

$C_{10}H_9N_3$
5-Amino-2,2′-bipyridine, A-1-00065

$C_{10}H_9N_3O_2$
N-(1*H*-Indole-3-carbonyl)urea, I-1-00014

$C_{10}H_{10}$
1-Phenylcyclobutene, P-1-00058

$C_{10}H_{10}Br_2O_2$
2,4-Bis(bromomethyl)benzoic acid; Me ester, *in* B-1-00126
2,5-Bis(bromomethyl)benzoic acid; Me ester, *in* B-1-00127
2,6-Bis(bromomethyl)benzoic acid; Me ester, *in* B-1-00128
3,4-Bis(bromomethyl)benzoic acid; Me ester, *in* B-1-00129
3,5-Bis(bromomethyl)benzoic acid; Me ester, *in* B-1-00130

$C_{10}H_{10}Br_2O_4S$
3,4-Bis(bromomethyl)-2,5-thiophenedicarboxylic acid; Di-Me ester, *in* B-1-00134

$C_{10}H_{10}N_2$
3(5)-Benzyl-1*H*-pyrazole, B-1-00072
4-Benzyl-1*H*-pyrazole, B-1-00073
1,3,4,5-Tetrahydropyrrolo[4,3,2-*de*]quinoline, T-1-00056

$C_{10}H_{10}N_2O_2$
5-Hydroxy-2-methylpyrazolo[1,5-*a*]pyridine; Ac, *in* H-1-00130
3-Phenyl-2,5-piperazinedione, P-1-00094

$C_{10}H_{10}N_2S_2$
2,4-Bis(methylthio)quinazoline, *in* Q-1-00001
2,4-Quinazolinedithiol; *N*,*N*′-Di-Me, *in* Q-1-00001

$C_{10}H_{10}O$
2-Phenylcyclopropanecarboxaldehyde, P-1-00061
Tricyclo[5.2.1.0^{2,6}]deca-2(6),8-dien-3-one, T-1-00170

$C_{10}H_{10}OS$
2,3-Dihydro-2-methyl-4*H*-1-benzothiopyran-4-one, D-1-00298
2,3-Dihydro-3-methyl-4*H*-1-benzothiopyran-4-one, D-1-00299
2,3-Dihydro-5-methyl-4*H*-1-benzothiopyran-4-one, D-1-00300
2,3-Dihydro-6-methyl-4*H*-1-benzothiopyran-4-one, D-1-00301
2,3-Dihydro-7-methyl-4*H*-1-benzothiopyran-4-one, D-1-00302
2,3-Dihydro-8-methyl-4*H*-1-benzothiopyran-4-one, D-1-00303
3,3-Dimethyl-1(3*H*)-isobenzofuranthione, D-1-00431
2-Methyl-2-propenethioic acid; *S*-Ph ester, *in* M-1-00121

$C_{10}H_{10}O_2$
4-Hydroxy-4-phenyl-2-butenal, H-1-00168
4-Methoxy-2-methylbenzofuran, *in* H-1-00105
4-Methoxy-3-methylbenzofuran, *in* H-1-00106
5-Methoxy-2-methylbenzofuran, *in* H-1-00109
1-Phenyl-1,2-butanedione, P-1-00054

$C_{10}H_{10}O_2S$
2,3-Dihydro-2-methyl-4*H*-1-benzothiopyran-4-one; *S*-Oxide, *in* D-1-00298
2,3-Dihydro-3-methyl-4*H*-1-benzothiopyran-4-one; *S*-Oxide, *in* D-1-00299
2,3-Dihydro-5-methyl-4*H*-1-benzothiopyran-4-one; *S*-Oxide, *in* D-1-00300
2,3-Dihydro-6-methyl-4*H*-1-benzothiopyran-4-one; *S*-Oxide, *in* D-1-00301
2,3-Dihydro-8-methyl-4*H*-1-benzothiopyran-4-one; *S*-Oxide, *in* D-1-00303

$C_{10}H_{10}O_3$
4,7-Dimethoxybenzo[*c*]furan, *in* D-1-00337
2-Oxiranylbenzoic acid; Me ester, *in* O-1-00035
4-Oxiranylbenzoic acid; Me ester, *in* O-1-00037

$C_{10}H_{10}O_3S$
2,3-Dihydro-2-methyl-4*H*-1-benzothiopyran-4-one; *S*,*S*-Dioxide, *in* D-1-00298
2,3-Dihydro-3-methyl-4*H*-1-benzothiopyran-4-one; *S*,*S*-Dioxide, *in* D-1-00299
2,3-Dihydro-5-methyl-4*H*-1-benzothiopyran-4-one; *S*,*S*-Dioxide, *in* D-1-00300
2,3-Dihydro-7-methyl-4*H*-1-benzothiopyran-4-one; *S*,*S*-Dioxide, *in* D-1-00302
2,3-Dihydro-8-methyl-4*H*-1-benzothiopyran-4-one; *S*,*S*-Dioxide, *in* D-1-00303
4,5,6,7-Tetrahydro-4-oxobenzo[*b*]thiophene-2-acetic acid, T-1-00049

$C_{10}H_{10}O_4$
4-(4-Hydroxyphenyl)-4-oxobutanoic acid, H-1-00171

$C_{10}H_{10}O_4S_2$
1*H*,3*H*-Thieno[3,4-*c*]thiophene-4,6-dicarboxylic acid; Di-Me ester, *in* T-1-00129

$C_{10}H_{11}Br_2$
1,3-Bis(2-bromoethyl)benzene, B-1-00123

$C_{10}H_{11}FN_2O_4$
2′,3′-Didehydro-2′,3′-dideoxy-2′-fluorothymidine, D-1-00213

$C_{10}H_{11}IO_2$
2-(2-Iodophenyl)ethanol; Ac, *in* I-1-00055

$C_{10}H_{11}N$
1*H*-1-Benzazepine; 2,3-Dihydro, *in* B-1-00001
3*H*-2-Benzazepine; 4,5-Dihydro, *in* B-1-00002

$C_{10}H_{11}NO$
3,4-Dihydro-1(2*H*)-isoquinolinone; *N*-Me, *in* D-1-00297
2,3-Dihydro-4(1*H*)-quinolinone; *N*-Me, *in* D-1-00328
2-Methyl-1*H*-indole-4-methanol, M-1-00074
3-Methyl-4-phenyl-2-azetidinone, M-1-00101
1,3,4,5-Tetrahydro-2*H*-1-benzazepin-2-one, T-1-00028
2,3,4,5-Tetrahydro-1*H*-2-benzazepin-1-one, T-1-00029

$C_{10}H_{11}NOS$
3,4-Dihydro-1,4-benzothiazepin-5(2*H*)-one; *N*-Me, *in* D-1-00260
2,3-Dihydro-2-methyl-4*H*-1-benzothiopyran-4-one; Oxime, *in* D-1-00298
2,3-Dihydro-3-methyl-4*H*-1-benzothiopyran-4-one; Oxime, *in* D-1-00299
2,3-Dihydro-8-methyl-4*H*-1-benzothiopyran-4-one; Oxime, *in* D-1-00303

$C_{10}H_{11}NO_2$
3,4-Dihydro-4-hydroxy-1(2*H*)-isoquinolinone; *N*-Me, *in* D-1-00283
3,4-Dihydro-5-methoxy-1(2*H*)-isoquinolinone, *in* D-1-00284
3,4-Dihydro-6-methoxy-1(2*H*)-isoquinolinone, *in* D-1-00285
3,4-Dihydro-7-methoxy-1(2*H*)-isoquinolinone, *in* D-1-00286
3,4-Dihydro-8-methoxy-1(2*H*)-isoquinolinone, *in* D-1-00287
3-Phenyl-2-azetidinecarboxylic acid, P-1-00044
1-Phenyl-1,2-butanedione; 2-Oxime, *in* P-1-00054

$C_{10}H_{11}NO_3$
5-Amino-4*H*-1,3-benzodioxin; *N*-Ac, *in* A-1-00055
1,3-Dihydro-3,3-dimethoxy-2*H*-indol-2-one, D-1-00269

$C_{10}H_{11}NO_4$
2-(Hydroxymethyl)-3-pyridinecarboxylic acid; Ac, Me ester, *in* H-1-00131
4-(Hydroxymethyl)-3-pyridinecarboxylic acid; Ac, Me ester, *in* H-1-00136
6-(Hydroxymethyl)-3-pyridinecarboxylic acid; Ac, Me ester, *in* H-1-00140

$C_{10}H_{11}N_3O_6$
5-Cyanouridine, *in* U-1-00007

$C_{10}H_{11}N_5$
2,4-Diamino-6-benzyl-1,3,5-triazine, D-1-00084

$C_{10}H_{11}N_{11}O_2$
2′,3′-Diazido-2′,3′-dideoxyadenosine, D-1-00115

$C_{10}H_{11}O_4P$
Phenylphosphinediacetic acid, P-1-00092

$C_{10}H_{12}$
1,4-Dimethylcubane, D-1-00380
1-Methyl-3-(2-propenyl)benzene, M-1-00122

$C_{10}H_{12}Br_2$
1,2-Bis(1-bromoethyl)benzene, B-1-00121
1,4-Bis(1-bromoethyl)benzene, B-1-00122

1,3-Bis(bromomethyl)-2,4-dimethylbenzene, B-1-00131
2,5-Bis(bromomethyl)-1,3-dimethylbenzene, B-1-00132

$C_{10}H_{12}ClNO_2$
2-[(2-Chloroethyl)amino]benzoic acid; Me ester, *in* C-1-00092

$C_{10}H_{12}FN_5O_4$
1-(3-Azido-2,3-dideoxy-2-fluoro-β-D-arabinofuranosyl)thymine, A-1-00251
2′-Deoxy-2′-fluoroguanosine, D-1-00027
3′-Deoxy-3′-fluoroguanosine, D-1-00028

$C_{10}H_{12}F_4O_6$
2-Deoxy-2-fluorolyxose; Trifluoromethyl glycoside, di-Ac, *in* D-1-00032
2-Deoxy-2-fluoroxylose; Trifluoromethyl glycoside, di-Ac, *in* D-1-00041

$C_{10}H_{12}N_2$
2,3-Dihydro-1*H*-cycloheptapyrazine; *N*-Me, *in* D-1-00263
1,2-Dihydro-1,2-dimethylphthalazine, *in* D-1-00306

$C_{10}H_{12}N_2O$
3,4-Dihydro-3,3-dimethyl-2(1*H*)-quinoxalinone, D-1-00272

$C_{10}H_{12}N_2O_2$
1-Phenyl-1,2-butanedione; Dioxime, *in* P-1-00054

$C_{10}H_{12}N_2O_4$
2,3′-Anhydrothymidine, A-1-00234

$C_{10}H_{12}N_2O_5$
4-*tert*-Butyl-2,6-dinitrophenol, B-1-00420

$C_{10}H_{12}N_2O_8$
5-Uridinecarboxylic acid, U-1-00007

$C_{10}H_{12}N_4O_4$
Hexahydro-4*a*,4*b*-dimethylcyclobuta[1,2-*d*:4,3-*d*′]dipyrimidine-2,4,5,7(3*H*,6*H*)-tetrone, H-1-00037

$C_{10}H_{12}O$
Cyclopropylphenylmethanol, C-1-00223
1-Phenylcyclobutanol, P-1-00056
3-Phenylcyclobutanol, P-1-00057
1-Phenylcyclopropanemethanol, P-1-00062
3*a*,4,7,7*a*-Tetrahydro-4,7-methano-1*H*-inden-1-ol, T-1-00040

$C_{10}H_{12}OS$
4-(Phenylthio)-2-butanone, *in* M-1-00008

$C_{10}H_{12}OSe$
2-Methylselenobenzoic acid; Et ester, *in* M-1-00130
4-Methylselenobenzoic acid; Et ester, *in* M-1-00132

$C_{10}H_{12}O_2$
Benzyl propionate, *in* P-1-00131
2′-Hydroxy-3′,4′-dimethylacetophenone, H-1-00077
2′-Hydroxy-3′,5′-dimethylacetophenone, H-1-00078
2′-Hydroxy-4′,5′-dimethylacetophenone, H-1-00079
2′-Hydroxy-4′,6′-dimethylacetophenone, H-1-00080
4-Hydroxy-2′,3′-dimethylacetophenone, H-1-00081
4′-Hydroxy-2′,5′-dimethylacetophenone, H-1-00082
4′-Hydroxy-2′,6′-dimethylacetophenone, H-1-00083
4′-Hydroxy-3′,5′-dimethylacetophenone, H-1-00084
5′-Hydroxy-2′,4′-dimethylacetophenone, H-1-00085
3-Hydroxy-1-phenyl-1-butanone, H-1-00167

$C_{10}H_{12}O_3$
4-(1-Hydroxyethyl)benzoic acid; Me ester, *in* H-1-00094

$C_{10}H_{12}O_4S_4$
2,3,6,7-Tetrakis(hydroxymethyl) tetrathiafulvalene, T-1-00073

$C_{10}H_{12}S$
1,2,3,4-Tetrahydro-1-naphthalenethiol, T-1-00047

$C_{10}H_{12}S_4$
Tetramethyltetrathiafulvalene, T-1-00090

$C_{10}H_{12}Se_4$
Tetramethyltetraselenafulvalene, T-1-00089

$C_{10}H_{13}BrO$
5-Bromo-2-adamantanone, B-1-00223

$C_{10}H_{13}BrO_6$
2-Bromo-2-deoxyaltrose; 1,6-Anhydro, 3,4-di-Ac, *in* B-1-00247

$C_{10}H_{13}ClNO_2P$
(4-Morpholinyl)phenylphosphinic acid; Chloride, *in* M-1-00137

$C_{10}H_{13}ClO_6$
2-Chloro-2-deoxyallose; 1,6-Anhydro, 3,4-di-Ac, *in* C-1-00035
3-Chloro-3-deoxyaltrose; 1,6-Anhydro, 2,4-di-Ac, *in* C-1-00038

$C_{10}H_{13}FN_2O_4$
1-(2,3-Dideoxy-2-fluoro-β-D-*threo*-pentofuranosyl)thymine, D-1-00217

$C_{10}H_{13}FO_6$
1,6-Anhydro-3-deoxy-3-fluoroidopyranose; Di-Ac, *in* A-1-00231
1,6-Anhydro-3-deoxy-3-fluoromannopyranose; Di-Ac, *in* A-1-00232

$C_{10}H_{13}F_8O_3P$
Bis(2,2,3,3-tetrafluoropropyl) (2-ethoxyethenyl) phosphonite, *in* E-1-00011

$C_{10}H_{13}NO$
1,2,3,4-Tetramethyl-5-nitrosobenzene, T-1-00085

$C_{10}H_{13}NO_2$
5-Amino-4*H*-1,3-benzodioxin; *N*,*N*-Di-Me, *in* A-1-00055
3-Amino-2-phenylpropanoic acid; Me ester, *in* A-1-00198
2′-Hydroxy-3′,5′-dimethylacetophenone; Oxime, *in* H-1-00078
2′-Hydroxy-4′,5′-dimethylacetophenone; Oxime, *in* H-1-00079

$C_{10}H_{13}NO_2S$
3,4-Dihydro-1*H*-2,3-benzothiazine; *N*-Et, *S*,*S*-dioxide, *in* D-1-00261

$C_{10}H_{13}NO_3$
2-Amino-2-benzyl-3-hydroxypropanoic acid, A-1-00060
2′-Amino-4′,5′-dimethoxyacetophenone, *in* A-1-00121
2-Amino-3-hydroxy-4-phenylbutanoic acid, A-1-00148
1-Nitro-2-adamantanone, N-1-00010

$C_{10}H_{13}NO_7$
2-β-D-Ribofuranosyl-4-oxazolecarboxylic acid; Me ester, *in* R-1-00003

$C_{10}H_{13}N_2O_7P$
Cyclic TMP, C-1-00186

$C_{10}H_{13}N_2O_8P$
Cyclic UMP; Me ester, *in* C-1-00187

$C_{10}H_{13}N_3O_6$
1,2,2-Trinitroadamantane, T-1-00252

$C_{10}H_{13}N_3O_7$
5-Uridinecarboxylic acid; Amide, *in* U-1-00007

$C_{10}H_{13}N_5O_4$
2′-Azido-2′,3′-dideoxy-5-methyluridine, A-1-00253

$C_{10}H_{13}O_2P$
Phenyl ethylvinylphosphinate, *in* E-1-00031

$C_{10}H_{13}O_4P$
Dimethyl (phenylacetyl)phosphonate, *in* P-1-00041

$C_{10}H_{13}O_5P$
Dimethyl (4-methoxybenzoyl)phosphonate, *in* M-1-00013

$C_{10}H_{13}O_6$
3,4-Dihydroxy-1*H*-pyrrole-2,5-dicarboxylic acid; Di-Me ether, Di-Me ester, *in* D-1-00353

$C_{10}H_{14}$
Tetracyclo[3.3.1.1^{3,7}.0^{1,3}]decane, T-1-00013

$C_{10}H_{14}Br_2O_5$
2-Bromo-2,6-dideoxytalopyranosyl bromide; Di-Ac, *in* B-1-00277

$C_{10}H_{14}Br_4O_2P_2$
1,3-Adamantanediphosphonic acid; Bis(dibromide), *in* A-1-00037

$C_{10}H_{14}Cl_2O_5$
2-Chloro-2,6-dideoxytalopyranosyl chloride; Di-Ac, *in* C-1-00074

$C_{10}H_{14}Cl_4O_2P_2$
1,3-Adamantanediphosphonic acid; Bis(dichloride), *in* A-1-00037

$C_{10}H_{14}F_2O_5$
2-Deoxy-2-fluorofucopyranosyl fluoride; Di-Ac, *in* D-1-00021

$C_{10}H_{14}NO_3P$
(4-Morpholinyl)phenylphosphinic acid, M-1-00137

$C_{10}H_{14}NO_3PS_2$
S,*S*-Diethyl (4-nitrophenyl)phosphonodithioate, *in* N-1-00029

$C_{10}H_{14}N_2O_4S$
4′-Thiothymidine, T-1-00135

$C_{10}H_{14}N_6O_5$
3,6-Diamino-1,5-dihydro-1-β-D-ribofuranosyl-4*H*-pyrazolo[3,4-*d*]pyrimidin-4-one, D-1-00103

$C_{10}H_{14}O$
3,8-Decadiyn-1-ol, D-1-00002
1,4-Dimethylbicyclo[2.2.2]oct-5-en-2-one, D-1-00373
1,5-Dimethylbicyclo[2.2.2]oct-5-en-2-one, D-1-00374

$C_{10}H_{14}O_2$
2,6-Dimethyl-1,4-benzenedimethanol, D-1-00371
Idramantone, H-1-00053
2-Methyl-1-phenyl-1,3-propanediol, M-1-00109
2-Methyl-3-phenyl-1,2-propanediol, M-1-00110

$C_{10}H_{14}O_2S$
tert-Butyl phenyl sulfone, *in* B-1-00433

$C_{10}H_{14}O_4$
Bicyclo[3.1.0]hexane-6,6-dicarboxylic acid; Di-Me ester, *in* B-1-00090
1,2-Bis(2-hydroxyethoxy)benzene, B-1-00173
Glycol dimethacrylate, G-1-00007

$C_{10}H_{14}O_6$
2,5:3,4-Dianhydroaltritol; 1,6-Di-Ac, *in* D-1-00111

$C_{10}H_{14}S$
tert-Butyl phenyl sulfide, B-1-00433

$C_{10}H_{14}S_4$
3,6,9,14-Tetrathiabicyclo[9.2.1]tetradeca-11,13-diene, T-1-00103

$C_{10}H_{15}BrO_6$
2-Bromo-2-deoxyarabinose; Me glycoside, 3,5-di-Ac, *in* B-1-00250
2-Bromo-2-deoxylyxose; Me glycoside, di-Ac, *in* B-1-00257
2-Bromo-2-deoxyxylose; Me glycoside, di-Ac, *in* B-1-00270
3-Bromo-3-deoxyxylose; Me glycoside, di-Ac, *in* B-1-00271
5-Bromo-5-deoxyxylose; Me glycoside, di-Ac, *in* B-1-00273

$C_{10}H_{15}Br_2P$
1-Adamantylphosphonous acid; Dibromide, *in* A-1-00041

(2-Methylphenyl)butanedioic acid; Anhydride, *in* M-1-00102
1-Oxo-2-indanecarboxylic acid; Me ester, *in* O-1-00046

$C_{11}H_{10}O_5$
5*a*,6,10,10*a*-Tetrahydro-1,4:6,10-diepoxy-2*H*-cyclohept[*d*]oxepin-5,9(1*H*,4*H*)dione, T-1-00033

$C_{11}H_{10}O_6$
2-Phenyl-1,1,1-ethanetricarboxylic acid, P-1-00069

$C_{11}H_{10}S$
2-Methyl-5-phenylthiophene, M-1-00114
3-Methyl-2-phenylthiophene, M-1-00115
4-Methyl-2-phenylthiophene, M-1-00116

$C_{11}H_{10}Te$
2-Methyl-1-benzotellurepin, M-1-00038

$C_{11}H_{11}Br$
1-Bromo-3-phenylbicyclo[1.1.1]pentane, B-1-00374

$C_{11}H_{11}BrO$
1-Bromo-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one, B-1-00390
3-Bromo-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one, B-1-00391
6-Bromo-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one, B-1-00392

$C_{11}H_{11}ClO$
1-Chloro-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one, C-1-00165
2-Chloro-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one, C-1-00166
3-Chloro-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one, C-1-00167
2-Indaneacetic acid; Chloride, *in* I-1-00011

$C_{11}H_{11}FN_2O_2$
5-Fluorotryptophan, F-1-00060
6-Fluorotryptophan, F-1-00061

$C_{11}H_{11}FO_3$
3-(4-Fluorophenyl)-2-oxopropanoic acid; Et ester, *in* F-1-00053

$C_{11}H_{11}F_3O_2$
3-(Trifluoromethyl)benzeneacetic acid; Et ester, *in* T-1-00191
4-(Trifluoromethyl)benzeneacetic acid; Et ester, *in* T-1-00192

$C_{11}H_{11}I$
1-Cyclopropyl-4-iodocubane, C-1-00222

$C_{11}H_{11}IN_2O_2$
5-Iodotryptophan, I-1-00066

$C_{11}H_{11}N$
1,3-Dimethylisoquinoline, D-1-00432
1,4-Dimethylisoquinoline, D-1-00433
1,5-Dimethylisoquinoline, D-1-00434
1,6-Dimethylisoquinoline, D-1-00435
1,7-Dimethylisoquinoline, D-1-00436
1,8-Dimethylisoquinoline, D-1-00437
3,4-Dimethylisoquinoline, D-1-00438
3,5-Dimethylisoquinoline, D-1-00439
3,6-Dimethylisoquinoline, D-1-00440
4,5-Dimethylisoquinoline, D-1-00441
4,7-Dimethylisoquinoline, D-1-00442
5,7-Dimethylisoquinoline, D-1-00443
5,8-Dimethylisoquinoline, D-1-00444
6,8-Dimethylisoquinoline, D-1-00445

$C_{11}H_{11}NO$
3-Amino-2-naphthalenemethanol, A-1-00185
1,4-Dimethylisoquinoline; *N*-Oxide, *in* D-1-00433
5,8-Dimethylisoquinoline; *N*-Oxide, *in* D-1-00444
1-Phenyl-2-propyn-1-amine; *N*-Ac, *in* P-1-00095

$C_{11}H_{11}NO_2$
1-Benzoyl-2-pyrrolidinone, B-1-00057
3-Benzoyl-2-pyrrolidinone, B-1-00058
5-Benzoyl-2-pyrrolidinone, B-1-00059
2,3-Dihydro-4(1*H*)-quinolinone; *N*-Ac, *in* D-1-00328
4-(4-Ethoxyphenyl)-4-oxobutanenitrile, *in* H-1-00171
1-Indolizinecarboxylic acid; Et ester, *in* I-1-00015
2-Methyl-1*H*-indole-3-acetic acid, M-1-00073
Phensuximide, *in* P-1-00096

$C_{11}H_{11}NO_2S$
2,3-Dihydro-2-thioxo-1*H*-indole-3-acetic acid; *N*-Me, *in* D-1-00332
2,3-Dihydro-2-thioxo-1*H*-indole-3-acetic acid; Me ester, *in* D-1-00332

$C_{11}H_{11}NO_3$
3,4-Dihydro-6-hydroxy-1(2*H*)-isoquinolinone; *O*-Ac, *in* D-1-00285
3,4-Dihydro-7-hydroxy-1(2*H*)-isoquinolinone; *O*-Ac, *in* D-1-00286

$C_{11}H_{11}NO_4$
3-Amino-6,7-dimethoxy-2*H*-1-benzopyran-2-one, *in* A-1-00123
2-Oxo-5-oxazolidinecarboxylic acid; Benzyl ester, *in* O-1-00048

$C_{11}H_{11}N_3O$
N-(1*H*-Imidazol-1-ylmethyl)benzamide, *in* A-1-00171

$C_{11}H_{12}$
Cyclopropylcubane, C-1-00221

$C_{11}H_{12}ClNO$
1-Chloro-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one; Oxime, *in* C-1-00165
2-Chloro-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one; Oxime, *in* C-1-00166
3-Chloro-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-one; Oxime, *in* C-1-00167

$C_{11}H_{12}N_2$
4-Benzyl-1-methyl-1*H*-pyrazole, *in* B-1-00073
1-Phenyl-1*H*-pyrrole-2-methanamine, *in* A-1-00182
1,3,4,5-Tetrahydropyrrolo[4,3,2-*de*]quinoline; 1-Me, *in* T-1-00056
1,3,4,5-Tetrahydropyrrolo[4,3,2-*de*]quinoline; 5-Me, *in* T-1-00056

$C_{11}H_{12}N_2O$
2,3-Dihydro-1*H*-pyrazolo[1,2-*b*]phthalazin-5(10*H*)-one, D-1-00325
2-Methyl-1*H*-indole-3-acetamide, *in* M-1-00073

$C_{11}H_{12}N_2O_2$
3-Methyl-6-phenyl-2,5-piperazinedione, M-1-00108

$C_{11}H_{12}O$
2,2-Dimethyl-1-indanone, D-1-00415
2,3-Dimethyl-1-indanone, D-1-00416
2,4-Dimethyl-1-indanone, D-1-00417
2,5-Dimethyl-1-indanone, D-1-00418
2,6-Dimethyl-1-indanone, D-1-00419
2,7-Dimethyl-1-indanone, D-1-00420
3,3-Dimethyl-1-indanone, D-1-00421
3,4-Dimethyl-1-indanone, D-1-00422
3,6-Dimethyl-1-indanone, D-1-00423
3,7-Dimethyl-1-indanone, D-1-00424
4,5-Dimethyl-1-indanone, D-1-00425
4,6-Dimethyl-1-indanone, D-1-00426
4,7-Dimethyl-1-indanone, D-1-00427
5,6-Dimethyl-1-indanone, D-1-00428
5,7-Dimethyl-1-indanone, D-1-00429
6,7-Dimethyl-1-indanone, D-1-00430
2-Phenyl-2-pentenal, P-1-00088

$C_{11}H_{12}O_2$
2-Benzoyltetrahydrofuran, B-1-00060
2-Indaneacetic acid, I-1-00011

$C_{11}H_{12}O_3$
1-(2,5-Dihydroxyphenyl)-3-methyl-2-buten-1-one, D-1-00350

$C_{11}H_{12}O_4$
2,3-Dihydro-6,7-dihydroxy-2,2-dimethyl-4*H*-1-benzopyran-4-one, D-1-00268
4-(4-Hydroxyphenyl)-4-oxobutanoic acid; Me ester, *in* H-1-00171
3-(3-Methoxy-4,5-methylenedioxyphenyl)-2-propen-1-ol, *in* T-1-00233
4-(4-Methoxyphenyl)-4-oxobutanoic acid, *in* H-1-00171
(2-Methylphenyl)butanedioic acid, M-1-00102
(4-Methylphenyl)butanedioic acid, M-1-00103

$C_{11}H_{12}S$
1-(Phenylthio)bicyclo[1.1.1]pentane, *in* B-1-00098

$C_{11}H_{13}NO$
3,3-Dimethyl-4-phenyl-2-azetidinone, D-1-00454
4-(Methoxymethyl)-2-methylindole, *in* M-1-00074
Pyrrolidine; *N*-Benzoyl, *in* P-1-00184

$C_{11}H_{13}NO_2$
3,4-Dihydro-6-methoxy-2-methyl-1(2*H*)-isoquinolinone, *in* D-1-00285
1,2,3,4,4*a*,10*a*-Hexahydro[1,4]benzodioxino[2,3-*c*]pyridine, H-1-00034
1,2,3,4-Tetrahydro-4-methyl-3-isoquinolinecarboxylic acid, T-1-00041
1,2,3,4-Tetrahydro-5-methyl-3-isoquinolinecarboxylic acid, T-1-00042

$C_{11}H_{13}NO_4$
2-(Hydroxymethyl)-3-pyridinecarboxylic acid; Ac, Et ester, *in* H-1-00131
3-(Hydroxymethyl)-2-pyridinecarboxylic acid; Ac, Et ester, *in* H-1-00133
6-(Hydroxymethyl)-2-pyridinecarboxylic acid; Ac, Et ester, *in* H-1-00139
6-(Hydroxymethyl)-3-pyridinecarboxylic acid; Ac, Et ester, *in* H-1-00140

$C_{11}H_{13}N_2O_9P$
Cyclic UMP; 2′-Ac, *in* C-1-00187

$C_{11}H_{14}ClNO_2$
4-[(2-Chloroethyl)amino]benzoic acid; Et ester, *in* C-1-00093

$C_{11}H_{14}FN_5O_2$
2′-Deoxy-2′-fluoro-*ara*-aristeromycin, D-1-00018

$C_{11}H_{14}F_3O_3P$
Diethyl [3-(trifluoromethyl)phenyl]phosphonate, *in* T-1-00185

$C_{11}H_{14}N_2$
2,3,5,10-Tetrahydro-1*H*-pyrazolo[1,2-*b*]phthalazine, T-1-00054

$C_{11}H_{14}N_2O_5$
5-*tert*-Butyl-2-methoxy-1,3-dinitrobenzene, *in* B-1-00420
2′,3′-Dideoxyuridine; 5′-Ac, *in* D-1-00220

$C_{11}H_{14}N_4O_4$
9-Deazaadenosine, D-1-00001

$C_{11}H_{14}O$
Cyclopropylmethoxyphenylmethane, *in* C-1-00223
1,2,3,4-Tetrahydro-1-methyl-2-naphthol, T-1-00043

$C_{11}H_{14}O_2$
2-Ethoxy-5-(1-propenyl)phenol, *in* P-1-00132
2′-Methoxy-3′,4′-dimethylacetophenone, *in* H-1-00077
2′-Methoxy-3′,5′-dimethylacetophenone, *in* H-1-00078
2′-Methoxy-4′,5′-dimethylacetophenone, *in* H-1-00079
2′-Methoxy-4′,6′-dimethylacetophenone, *in* H-1-00080
4′-Methoxy-2′,3′-dimethylacetophenone, *in* H-1-00081
4′-Methoxy-2′,5′-dimethylacetophenone, *in* H-1-00082
4′-Methoxy-2′,6′-dimethylacetophenone, *in* H-1-00083
4′-Methoxy-3′,5′-dimethylacetophenone, *in* H-1-00084
5′-Methoxy-2′,4′-dimethylacetophenone, *in* H-1-00085

2-Bromodiphenylmethane, B-1-00288
3-Bromodiphenylmethane, B-1-00289
3-Bromo-2-methyl-1,1′-biphenyl, B-1-00315

$C_{13}H_{11}BrO$
2-Bromodiphenylmethanol, B-1-00290
3-Bromodiphenylmethanol, B-1-00291

$C_{13}H_{11}ClO$
2-Chlorodiphenylmethanol, C-1-00089
3-Chlorodiphenylmethanol, C-1-00090

$C_{13}H_{11}F$
2-Fluoro-2′-methylbiphenyl, F-1-00030
2-Fluoro-3-methylbiphenyl, F-1-00031
2-Fluoro-3′-methylbiphenyl, F-1-00032
2-Fluoro-4-methylbiphenyl, F-1-00033
2-Fluoro-4′-methylbiphenyl, F-1-00034
3-Fluoro-2-methylbiphenyl, F-1-00035
3′-Fluoro-2-methylbiphenyl, F-1-00036
3-Fluoro-3′-methylbiphenyl, F-1-00037
3-Fluoro-4-methylbiphenyl, F-1-00038
3-Fluoro-4′-methylbiphenyl, F-1-00039
4′-Fluoro-2-methylbiphenyl, F-1-00040
4′-Fluoro-3-methylbiphenyl, F-1-00041
4-Fluoro-4′-methylbiphenyl, F-1-00042

$C_{13}H_{11}FO$
2-Fluorodiphenylmethanol, F-1-00015
3-Fluorodiphenylmethanol, F-1-00016
4-Fluorodiphenylmethanol, F-1-00017

$C_{13}H_{11}F_2OP$
(Difluoromethyl)diphenylphosphine; Oxide, *in* D-1-00241
Methyl bis(3-fluorophenyl)phosphinite, *in* B-1-00166
Methyl bis(4-fluorophenyl)phosphinite, *in* B-1-00167

$C_{13}H_{11}F_2P$
(Difluoromethyl)diphenylphosphine, D-1-00241

$C_{13}H_{11}N$
3,4-Dihydroacridine, D-1-00257

$C_{13}H_{11}NO$
3-Hydroxy-1-methyl-9*H*-carbazole, H-1-00116
3-Hydroxy-2-methyl-9*H*-carbazole, H-1-00117
3-Hydroxy-5-methyl-9*H*-carbazole, H-1-00118
3-Hydroxy-7-methyl-9*H*-carbazole, H-1-00119
3-Hydroxy-8-methyl-9*H*-carbazole, H-1-00120

$C_{13}H_{11}NO_2$
1,4-Dihydrocyclopent[*b*]indol-3(2*H*)-one; *N*-Ac, *in* D-1-00265

$C_{13}H_{11}NO_3S$
3-Benzoylbenzenesulfonic acid; Amide, *in* B-1-00041
4-Benzoylbenzenesulfonic acid; Amide, *in* B-1-00042

$C_{13}H_{11}NS$
3-(2-Thienyl)-1*H*-indole; *N*-Me, *in* T-1-00131

$C_{13}H_{11}O_2P$
Diphenylphosphinecarboxylic acid, D-1-00507
9*H*-Fluoren-9-ylphosphonous acid, F-1-00005

$C_{13}H_{12}$
1-Methylacenaphthene, M-1-00016
3-Methylacenaphthene, M-1-00017
4-Methylacenaphthene, M-1-00018
5-Methylacenaphthene, M-1-00019
1-(1-Propenyl)naphthalene, P-1-00133
2-(1-Propenyl)naphthalene, P-1-00134

$C_{13}H_{12}BrCl_2N_3O$
▶ Bromuconazole, B-1-00406

$C_{13}H_{12}FOP$
(Fluoromethyl)diphenylphosphine; Oxide, *in* F-1-00043

$C_{13}H_{12}FP$
(Fluoromethyl)diphenylphosphine, F-1-00043

$C_{13}H_{12}F_3NO_2$
7-Ethylamino-6-methyl-4-trifluoromethylcoumarin, *in* A-1-00184

$C_{13}H_{12}N_4$
▶ 2-Amino-3-methyl-6-phenyl-3*H*-imidazo[4,5-*b*]pyridine, *in* A-1-00195
▶ 1-Methyl-6-phenyl-1*H*-imidazo[4,5-*b*]pyridin-2-amine, *in* A-1-00195

$C_{13}H_{12}O$
1-Acenaphthenemethanol, A-1-00002

$C_{13}H_{12}OSe_2$
3,4-Dihydro-2*H*-naphtho[1,8-*bc*]-1,5-diselenocin; Monoxide, *in* D-1-00312

$C_{13}H_{12}O_2$
1,2,3,4-Tetrahydroxanthone, T-1-00058

$C_{13}H_{12}O_3$
8-Hydroxy-1-naphthalenemethanol; 1′-Ac, *in* H-1-00155

$C_{13}H_{12}O_5$
4-Hydroxy-5,7-dimethoxy-2-naphthalenecarboxylic acid, *in* T-1-00230

$C_{13}H_{12}S$
2,3-Dihydro-1*H*-naphtho[2,1-*b*]thiopyran, D-1-00313
3,4-Dihydro-2*H*-naphtho[1,2-*b*]thiopyran, D-1-00314

$C_{13}H_{12}S_2$
Benzyl phenyl disulfide, B-1-00070

$C_{13}H_{12}Se_2$
Bis(phenylseleno)methane, B-1-00197
3,4-Dihydro-2*H*-naphtho[1,8-*bc*]-1,5-diselenocin, D-1-00312

$C_{13}H_{13}NO$
1-(1*H*-Indol-3-yl)-3-methyl-2-buten-1-one, I-1-00022

$C_{13}H_{13}NO_2$
1-Methyl-3-isoquinolinecarboxylic acid; Et ester, *in* M-1-00078

$C_{13}H_{13}NO_5$
3-(Acetylamino)-6,7-dimethoxycoumarin, *in* A-1-00123

$C_{13}H_{13}O_3P$
(Diphenylmethyl)phosphonic acid, D-1-00504

$C_{13}H_{14}N_2O_2$
3-Amino-1,2,3,4-tetrahydro-3-carbazolecarboxylic acid, A-1-00209

$C_{13}H_{14}O_2$
3-Phenyl-3-cyclohexene-1-carboxylic acid, P-1-00059

$C_{13}H_{15}BrO_5$
3-Bromo-3-deoxyarabinose; Me glycoside, 5-benozyl, *in* B-1-00251
2-Bromo-2-deoxyxylose; Me glycoside, 3-benzoyl, *in* B-1-00270
2-Bromo-2-deoxyxylose; Me glycoside, 5-benzoyl, *in* B-1-00270

$C_{13}H_{15}FO_4$
1,6-Anhydro-3-deoxy-3-fluoroaltropyranose; 4-Benzyl, *in* A-1-00230

$C_{13}H_{15}IO_4$
5-Deoxy-5-iodoribose; Me glycoside, 2,3-*O*-benzylidene, *in* D-1-00066

$C_{13}H_{15}IO_5$
2-Deoxy-2-iodoarabinose; Me glycoside, 4-benzoyl, *in* D-1-00049
3-Deoxy-3-iodoarabinose; Me glycoside, 5-benzoyl, *in* D-1-00050
3-Deoxy-3-iodoxylose; Me glycoside, 4-benzoyl, *in* D-1-00072

$C_{13}H_{15}NO_3$
5-Oxo-3-pyrrolidinecarboxylic acid; *N*-Benzyl, Me ester, *in* O-1-00054

$C_{13}H_{16}$
1-Phenylbicyclo[2.2.1]heptane, P-1-00050
7-Phenylbicyclo[2.2.1]heptane, P-1-00051

$C_{13}H_{16}ClP$
(1-Methylpropadienyl)(2,4,6-trimethylphenyl) phosphinous chloride, M-1-00120

$C_{13}H_{16}FN_3O_5$
2′,3′-Dideoxy-2′-fluorocytidine; 2′-Epimer, di-Ac, *in* D-1-00215

$C_{13}H_{16}F_4O_8$
2-Deoxy-2-fluorotalose; Trifluoromethyl glycoside, tri-Ac, *in* D-1-00037

$C_{13}H_{16}N_2O_2$
3-Aminohexahydro-2*H*-azepin-2-one; *N*-Benzoyl, *in* A-1-00142

$C_{13}H_{16}O_2$
1-Benzoylcyclohexanol, B-1-00048

$C_{13}H_{16}O_3$
1-(2,5-Dimethoxyphenyl)-3-methyl-2-buten-1-one, *in* D-1-00350
2-Hydroxy-2-phenylcyclohexanecarboxylic acid, H-1-00169

$C_{13}H_{16}O_4$
2,3-Dihydro-6,7-dimethoxy-2,2-dimethyl-4*H*-1-benzopyran-4-one, *in* D-1-00268
(2-Methylphenyl)butanedioic acid; Di-Me ester, *in* M-1-00102
(4-Methylphenyl)butanedioic acid; Di-Me ester, *in* M-1-00103

$C_{13}H_{17}BrO_4$
3-Bromo-3-deoxyxylose; Benzyl glycoside, 2-Me, *in* B-1-00271
3-Bromo-3-deoxyxylose; Benzyl glycoside, 4-Me, *in* B-1-00271

$C_{13}H_{17}FO_4$
2-Deoxy-2-fluoroxylose; Me glycoside, 5-benzyl, *in* D-1-00041

$C_{13}H_{17}NO_3$
2-Amino-2-ethyl-3-phenylpropanoic acid; *N*-Ac, *in* A-1-00134

$C_{13}H_{18}$
Benzylcyclohexane, B-1-00063

$C_{13}H_{18}NO_7P$
Amino(dimethoxyphosphinyl)acetic acid; *N*-Benzyloxycarbonyl, Me ester, *in* A-1-00125

$C_{13}H_{18}O_3$
4-(1-Hydroxyethyl)benzoic acid; Butyl ester, *in* H-1-00094

$C_{13}H_{19}Br$
1-Bromo-7-phenylheptane, B-1-00376

$C_{13}H_{19}BrO_8$
2-Bromo-2-deoxymannose; Me glycoside, tri-Ac, *in* B-1-00261
6-Bromo-6-deoxymannose; Me glycoside, tri-Ac, *in* B-1-00262
4-Bromo-4-deoxytagatose; Me glycoside, tri-Ac, *in* B-1-00267
4-Bromo-4-deoxytalose; Me glycoside, tri-Ac, *in* B-1-00268

$C_{13}H_{19}Cl$
1-Chloro-7-phenylheptane, C-1-00152

$C_{13}H_{19}ClO_8$
3-Chloro-3-deoxyaltrose; Me glycoside, tri-Ac, *in* C-1-00038
1-Chloro-1-deoxyfructose; Me glycoside, tri-Ac, *in* C-1-00042
2-Chloro-2-deoxymannose; Me glycoside, tri-Ac, *in* C-1-00052

$C_{13}H_{19}IO_6S_2$
5-Deoxy-5-iodoarabinose; Ethylene dithioacetal, 2,3,4-tri-Ac, *in* D-1-00051

$C_{13}H_{19}IO_8$
6-Deoxy-6-iodoallose; Me glycoside, tri-Ac, *in* D-1-00045
2-Deoxy-2-iodoaltrose; Me glycoside, tri-Ac, *in* D-1-00046
4-Deoxy-4-iodofructose; Me glycoside, tri-Ac, *in* D-1-00052
2-Deoxy-2-iodomannose; Me glycoside, tri-Ac, *in* D-1-00060
6-Deoxy-6-iodomannose; Me glycoside, tri-Ac, *in* D-1-00061
2-Deoxy-2-iodotalose; Me glycoside, tri-Ac, *in* D-1-00069

3-Bromo-3-deoxylyxose; Me glycoside, dibenzoyl, *in* B-1-00258
2-Bromo-2-deoxyribose; Me glycoside, dibenzoyl, *in* B-1-00264
5-Bromo-5-deoxyribose; Me glycoside, 2,3-dibenzoyl, *in* B-1-00265
2-Bromo-2-deoxyxylose; Me glycoside, dibenzoyl, *in* B-1-00270
3-Bromo-3-deoxyxylose; Me glycoside, dibenzoyl, *in* B-1-00271
4-Bromo-4-deoxyxylose; Me glycoside, dibenzoyl, *in* B-1-00272

$C_{20}H_{19}FO_6$
Xylofuranosyl fluoride; 2-Me, 3,5-dibenzoyl, *in* X-1-00002
Xylopyranosyl fluoride; 2-Me, 3,4-dibenzoyl, *in* X-1-00003

$C_{20}H_{19}IO_6$
3-Deoxy-3-iodoribose; Me glycoside, 2,4-dibenzoyl, *in* D-1-00065

$C_{20}H_{20}Br_2O_3$
Bromethirin, B-1-00222

$C_{20}H_{21}FO_5$
2-Deoxy-2-fluoroxylose; Me glycoside, 3-benzoyl, 5-benzyl, *in* D-1-00041

$C_{20}H_{21}IO_5$
2-Deoxy-2-iodotalose; Benzyl glycoside, 4,6-*O*-benzylidene (*S*-), *in* D-1-00069

$C_{20}H_{22}O_2$
1,2-Bis(4-hydroxyphenyl)acetylene; Diisopropyl ether, *in* B-1-00182
1,2-Bis(4-hydroxyphenyl)acetylene; Dipropyl ether, *in* B-1-00182

$C_{20}H_{22}O_3$
Avobenzone, A-1-00239

$C_{20}H_{22}O_{12}$
Methoxytunicoside, *in* H-1-00100

$C_{20}H_{23}ClO_4$
2-Chloro-2-deoxyarabinose; Me glycoside, 3,5-dibenzyl, *in* C-1-00039

$C_{20}H_{24}O_3$
16,17-Epoxyestra-1,3,5(10)-trien-3-ol; Ac, *in* E-1-00007

$C_{20}H_{24}S_2$
2,5,7,10-Tetraisopropylidene-1,6-dithia-3,8-cyclodecadiyne, T-1-00062

$C_{20}H_{25}ClO_2$
Butethrin, B-1-00410

$C_{20}H_{25}NO_9$
3-Amino-3-deoxymannose; Me glycoside, *N*-benzoyl, 2,4,6-tri-Ac, *in* A-1-00106

$C_{20}H_{26}$
[2.2](1,3)Adamantanoparacyclophane, A-1-00038

$C_{20}H_{28}$
1-Decylnaphthalene, D-1-00012
2-Decylnaphthalene, D-1-00013

$C_{20}H_{28}N_2$
11,12-Bis(diethylamino)nonatriafulvalene, B-1-00149

$C_{20}H_{28}OP_2$
1,2-Di-*tert*-butyl-1,2-diphenyldiphosphine; Monoxide, *in* D-1-00169

$C_{20}H_{28}O_2P_2$
1,2-Di-*tert*-butyl-1,2-diphenyldiphosphine; 1,2-Dioxide, *in* D-1-00169

$C_{20}H_{28}O_5$
11,17-Dihydroxy-3-oxo-4-androstene-17-carboxylic acid, D-1-00349

$C_{20}H_{28}P_2$
1,2-Di-*tert*-butyl-1,2-diphenyldiphosphine, D-1-00169

$C_{20}H_{31}OP$
Di-1-adamantylphosphine; Oxide, *in* D-1-00082

$C_{20}H_{31}P$
Di-1-adamantylphosphine, D-1-00082

$C_{20}H_{31}PS$
Di-1-adamantylphosphine; Sulfide, *in* D-1-00082

$C_{20}H_{31}PSe$
Di-1-adamantylphosphine; Selenide, *in* D-1-00082

$C_{20}H_{32}O_4$
Ostopanic acid; Et ester, *in* D-1-00492

$C_{20}H_{35}OPS_2$
O-Ethyl (2,4,6-tri-*tert*-butylphenyl) phosphonodithioate, *in* T-1-00156

$C_{20}H_{36}OP_4$
1,3,5,7-Tetra-*tert*-butyl-1,3,5,7-tetraphosphacubane; Monoxide, *in* T-1-00006

$C_{20}H_{36}P_4$
1,3,5,7-Tetra-*tert*-butyl-1,3,5,7-tetraphosphacubane, T-1-00006

$C_{20}H_{38}O_2$
4-Eicosenoic acid, E-1-00004

$C_{20}H_{40}$
10-Eicosene, E-1-00003

$C_{20}H_{42}O_2$
1,20-Eicosanediol, E-1-00002

$C_{20}H_{43}O_3P$
Dibutyl dodecylphosphonate, *in* D-1-00552

$C_{21}H_{12}$
2,3:6,7:10,11-Tricyclopropatriphenylene, T-1-00174

$C_{21}H_{12}O$
12*H*-Dibenzo[*b*,*h*]fluoren-12-one, D-1-00128

$C_{21}H_{14}O_2$
2,2-Diphenyl-1,3-indanedione, D-1-00501

$C_{21}H_{15}N_3$
4′-Phenyl-4,2′:6′,4″-terpyridine, P-1-00100

$C_{21}H_{16}$
1,3,3-Triphenyl-1-propyne, T-1-00263

$C_{21}H_{18}IO_2P$
Methyl iodo(triphenylphosphoranylidene) acetate, *in* I-1-00065

$C_{21}H_{18}OS$
Triphenylmethanethiol; *S*-Ac, *in* T-1-00261

$C_{21}H_{18}O_3$
4-(4-Biphenylyloxy)benzoic acid; Et ester, *in* B-1-00114

$C_{21}H_{19}BrO_7$
5-Bromo-5-deoxyribose; 2,3-Dibenzoyl, 1-Ac, *in* B-1-00265
2-Bromo-2-deoxyxylose; 1,3-Dibenzoyl, 4-Ac, *in* B-1-00270

$C_{21}H_{19}IO_7$
5-Deoxy-5-iodoribose; 2,3-Dibenzoyl, 1-Ac, *in* D-1-00066

$C_{21}H_{21}BrO_6$
3-Bromo-3-deoxyaltrose; Me glycoside, 4,6-*O*-benzylidene, 2-benzoyl, *in* B-1-00248

$C_{21}H_{21}BrO_7$
6-Bromo-6-deoxymannose; Me glycoside, 2,3-dibenzoyl, *in* B-1-00262

$C_{21}H_{21}ClO_6$
2-Chloro-2-deoxymannose; Me glycoside, 4,6-*O*-benzylidene (*R*-), 3-benzoyl, *in* C-1-00052

$C_{21}H_{23}NO_6$
3-Amino-3-deoxymannose; Me glycoside, 4,6-*O*-benzylidene, *N*-benzoyl, *in* A-1-00106

$C_{21}H_{24}$
1,2,3,4,5,6,7,8,9,10,11,12-Dodecahydro[1,4:5,8:9,12] trimethanotriphenylene, D-1-00547

$C_{21}H_{25}IO_5$
6-Deoxy-6-iodoaltrose; Me glycoside, 2,3-dibenzyl, *in* D-1-00048

$C_{21}H_{25}IO_7S$
6-Deoxy-6-iodogulose; Me glycoside, 3-benzyl, 2-tosyl, *in* D-1-00055

$C_{21}H_{25}NO_4$
2-Amino-2-benzyl-3-phenylpropanoic acid; *N*-*tert*-Butoxycarbonyl, *in* A-1-00062

$C_{21}H_{25}NO_{10}$
3-Amino-3-deoxymannose; *N*-Benzoyl, 1,2,4,6-tetra-Ac, *in* A-1-00106

$C_{21}H_{27}NO_2P_2$
3,4-Bis(phenylphosphino)pyrrolidine; 1-*tert*-Butoxycarbonyl, *in* B-1-00196

$C_{21}H_{28}O_3$
▶ Pregn-4-ene-3,11,20-trione, P-1-00127

$C_{21}H_{28}O_{12}$
Cistanoside I, *in* R-1-00002

$C_{21}H_{29}N_2P$
N,*N*,*N*′,*N*′-Tetraethyl-*P*-9*H*-fluoren-9-ylphosphonous diamide, *in* F-1-00005

$C_{21}H_{29}O_3P$
Bis(1,1-dimethylethyl) (diphenylmethyl) phosphonate, *in* D-1-00504

$C_{21}H_{30}$
1-Undecylnaphthalene, U-1-00004
2-Undecylnaphthalene, U-1-00005

$C_{21}H_{30}O$
2,2′-Biadamantyl ketone, B-1-00079

$C_{21}H_{30}O_5$
Cortienic acid; Me ester, *in* D-1-00349

$C_{21}H_{33}OP$
Di-1-adamantylmethylphosphine; Oxide, *in* D-1-00081

$C_{21}H_{33}P$
Di-1-adamantylmethylphosphine, D-1-00081

$C_{21}H_{34}IP$
Di-1-adamantyl(methyl)phosphonium iodide, *in* D-1-00082

$C_{21}H_{38}O_6$
8,16-Dihydroxyhexadecanoic acid; Me ester, di-Ac, *in* D-1-00343

$C_{21}H_{39}BF_4P_4$
1,3,5,7-Tetra-*tert*-butyl-1,3,5,7-tetraphosphacubane; Monomethotetrafluoroborate, *in* T-1-00006

$C_{21}H_{46}BrN$
Trimethyloctadecylammonium(1+); Bromide, *in* T-1-00245

$C_{21}H_{46}ClN$
Trimethyloctadecylammonium chloride, *in* T-1-00245

$C_{21}H_{46}IN$
Trimethyloctadecylammonium(1+); Iodide, *in* T-1-00245

$C_{21}H_{46}N^{\oplus}$
Trimethyloctadecylammonium(1+), T-1-00245

$C_{22}H_9O_3^{3\ominus}$
4,8,12-Trioxodibenzo[*cd*,*mn*]pyrenediyl(3−), T-1-00255

$C_{22}H_{10}O_3$
1*H*,3*H*-Perylo[3,4-*cd*]pyran-1,3-dione, *in* P-1-00032

$C_{22}H_{12}$
Biphenyleno[2,1-*a*]biphenylene, B-1-00108
Biphenyleno[2,3-*a*]biphenylene, B-1-00109
Biphenyleno[2,3-*b*]biphenylene, B-1-00110
Triangulene, T-1-00143

$C_{22}H_{12}N_4$
Naphtho[1,2-*c*:5,6-*c*′]dicinnoline, N-1-00004

$C_{22}H_{12}O_4$
3,4-Perylenedicarboxylic acid, P-1-00032

Chemical Abstracts Service Registry Number Index

This index lists in numerical order all Chemical Abstracts Service (CAS) registry numbers contained in the Dictionary.

The first digit of the Dictionary Number refers to the number of the Supplement in which the Entry appears. In this, the First Supplement, the first digit is invariably 1.

Where a CAS registry number applies to a derivative or to a stereoisomer or other variant embedded within the entry, the Dictionary number is preceded by the word '*in*'.

The symbol ▶ preceding an index term indicates that the Dictionary Entry contains information on toxic or hazardous properties.

The symbol † refers to a name which is known to be a duplicated name.

CAS Registry Number Index