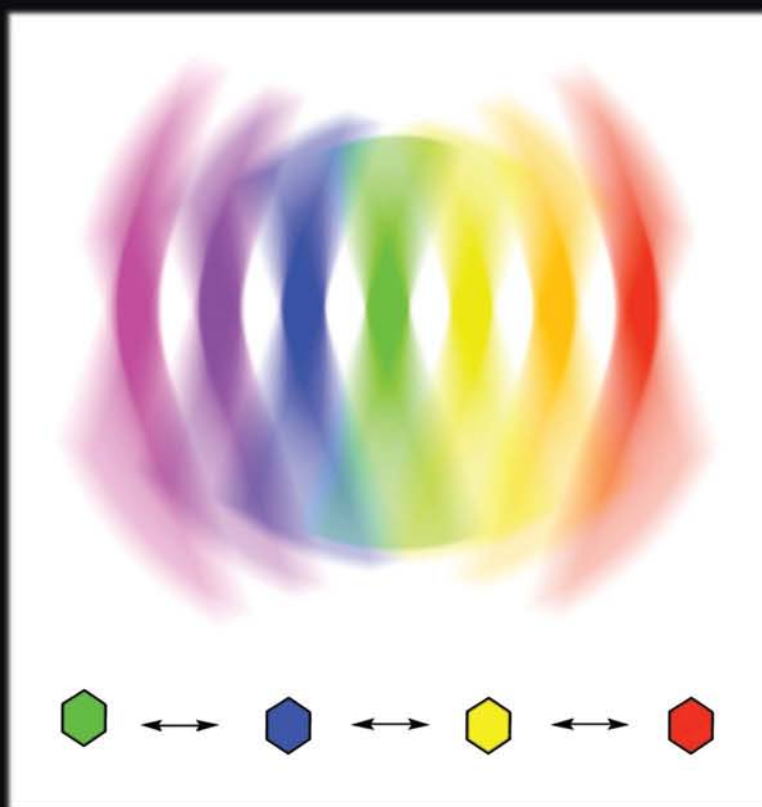


# HANDBOOK OF ACID-BASE INDICATORS

R. W. SABNIS



HANDBOOK OF  
**ACID-BASE**  
**INDICATORS**



# HANDBOOK OF ACID-BASE INDICATORS

**R. W. SABNIS**

Squire, Sanders & Dempsey LLP  
San Francisco, U.S.A.



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# *Dedication*

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*to*

*My Guru/Mentor/Advisor*

**Prof. D. W. Rangnekar**



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# Preface

Color change has been a fascination of individuals for a long time. The two major types of dyes which are traditionally used for color change are leuco dyes and acid–base indicators. Leuco dyes are of limited use because three components are required to effect the color change transition. Generally, a color former (the leuco dye), a developer (such as phenolic compound) and a reversible matrix (such as a long chain alcohol) are combined. An often noted drawback with leuco dye systems is their water insolubility, thus, leuco dyes can only be used in solvent-based systems. Very few leuco dyes are commercially available. The synthetic methods of leuco dyes are complex, involve multiple steps, and do not generate high yields.

Acid–base indicators are also commonly known as pH indicators. Acid–base indicators are substances (dyes) which change color with pH. They are usually weak acids or bases, which when dissolved in water dissociate slightly and form ions. The major benefits of acid–base indicators over leuco dyes include: (a) acid–base indicators are one-component systems compared to three components required for a color change in leuco dye system; (b) acid–base indicators are generally soluble in organic solvent; they can be dissolved in water by making sodium or potassium salts and thus can be used in aqueous as well as solvent based systems; (c) acid–base indicators are commercially available or can be synthesized in excellent yield and purity.

There is no book available in the market directly on acid–base indicators even though use of acid–base indicators is widespread, growing rapidly and has exploded in the past two decades. There was a need to publish a book that provided an immediate incentive for compiling the notes to update the scientific community with the wealth of information on acid–base indicators. The literature in dyestuff chemistry, particularly on acid–base indicators, is largely in patents. This book provides a systematic and up-to-date library of information on 200+ acid–base indicators as a reference handbook. It was compiled as a resource guide for chemists and non-chemists in industry and university.

Acid–base indicators are arranged alphabetically by the most commonly used name. Again, the choice of primary name is somewhat arbitrary, but an effort has been made to strike a balance between names that are easily recognizable and names that are chemically informative. The detailed information of each acid–base indicator is covered in the following order: common name, other names, CA index name, CAS registry number, Merck index number (Merck Index 14th Edition, 2006), chemical structure, chemical/dye class, molecular formula, molecular weight, pH range, color change at pH, pKa, physical form, solubility, UV-visible ( $\lambda_{\text{max}}$ ), melting point, boiling point, synthesis, major applications, safety/toxicity, and references of 200+ acid–base indicators. Where there are discrepancies between different values, the author used his judgment on selecting the most likely value.

Numerous recent references have been provided on various synthetic methods, major applications and safety/toxicity data. Space and format limitations prevent giving all the references for each indicator. This is the first book that provides safety/toxicity data with reference to acute toxicity, aquatic toxicity, carcinogenicity, cytotoxicity, ecotoxicity, genotoxicity, hemotoxicity, hepatotoxicity, mutagenicity, neurotoxicity, oral toxicity, phototoxicity, and phytotoxicity, and so forth.

Omissions as well as errors of fact and interpretation are inevitable in dealing with a vast subject such as acid–base indicators. I shall be glad to have my attention drawn to errors and to incorporate suggestions for improvement when a revision becomes possible.

I express my profound respect to my late-father, Wasudeo and late-mother, Suhasini who strained every resource to educate me. Words are inadequate to express my sincere appreciation to my wife

Madhuri and daughter Anika. It would not have been possible to write this book without their encouragement and patience. It is a great pleasure to express my gratitude and appreciation to CRC Press LLC (Taylor & Francis Group PLC) for giving me an opportunity to write this book.

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# Author

**Ram W. Sabnis** is currently a patent agent at Squire, Sanders & Dempsey L.L.P. in San Francisco, California, USA. His interests include dyes, pigments, organic chemistry, heterocycles, polymers, synthesis, formulations, coatings, displays, semiconductors, nanotechnology, biotechnology, medicinal chemistry, medical devices and patents. Presently, he focuses on writing and prosecuting U.S. and international patents, patentability opinions, and providing strong technical support. He is a registered patent agent with the U.S. Patent & Trademark Office (USPTO) and is also the inventor of more than 50 U.S. and international patents (issued/published). Prior to entering the legal (patents) field, he was a research chemist for Ascadia, General Electric, Brewer Science, U.S. Textiles and Invitrogen.



Dr Sabnis was born and raised in Mumbai, India. He received his M.Sc. in organic chemistry from University of Mumbai and Ph.D. in organic chemistry (Dyes) from University Institute of Chemical Technology (UICT), University of Mumbai, India. He is a fellow of the American Institute of Chemists, USA. He was awarded a chartered colourist and fellow of the Society of Dyers & Colourists, U.K.

Dr. Sabnis is one of the world's foremost experts in dyes, inventing the world's first colored bubbles (non-staining) and color changing dye system with many applications. He has more than 25 years of industrial and academic research experience in dye chemistry, particularly, dyes for biomedical (fluorescent probes), personal care products, health/beauty products, displays, inks, paints, plastics, textiles, and toys applications. He has written over 150 publications which include books, book chapters, patents, reviews, papers, and symposia presentations. Dr. Sabnis is a recipient of the Perkin Innovation Award by Society of Dyers & Colourist, U.K.; Grand Innovation Award by Popular Science, U.S.; Six Sigma Green Belt & Competitive Spirit Award by GE, U.S.; Best Doctoral Thesis Award by University of Mumbai, India. He will continue to focus his activities on fascinating dye chemistry as well as demanding intellectual property in the years to come.





# A

# A

## ACID ALIZARIN VIOLET N

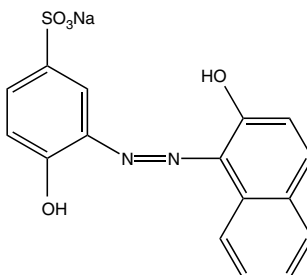
**Other Names** C.I. Mordant Violet 5; C.I. Mordant Violet 5, monosodium salt; Eriochrome Violet B; Acid Alizarin Violet N; Acid Alizarine Violet; Acid Alizarine Violet B; Acid Chrome Violet K; Acid Chrome Violet N; Aizen Chrome Violet BH; Alizarine Violet N; Alphacroic Violet B; Atlantichrome Violet B; Brasilan Chrome Violet B; C.I. 15670; Chromacid Violet R; Chromaven Violet B; Chrome Fast Violet B; Chrome Violet B; Chrome Violet K; Chrome Violet R; Cromal Violet B; Diacromo Violet N; Diamond Corinth N; Durochrome Violet B; Erio Chrome Violet BA; Erio Chrome Violet BR; Hispacrom Violet B; Java Chrome Violet B; Magracrom Violet N; Mitsui Chrome Violet BC; Monochrome Violet B; Mordant Violet 5; Omega Chrome Dark Violet D; Pontachrome Violet SW; Solochrome Violet; Solochrome Violet R; Solochrome Violet RS; Solocrom Violet RS; Sunchromine Violet B; Superchrome Violet B; Symulon Chrome Violet B; Tetrochrome Violet N; Yodochrome Violet B

**CA Index Name** Benzenesulfonic acid, 4-hydroxy-3-[(2-hydroxy-1-naphthalenyl)azo]-, monosodium salt

**CAS Registry Number** 2092-55-9

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{16}H_{11}N_2O_5SNa$

**Molecular Weight** 366.33

**pH Range** 6.5–9.0

**Color Change at pH** Orange-red (6.5) to violet (9.0)

**pKa** 4.35, 7.4, 9.35

**Physical Form** Reddish-violet crystals

**Solubility** Soluble in water, ethanol

**UV-Visible** ( $\lambda_{max}$ ) 501 nm

**Melting Point** >300°C

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** inks,<sup>4</sup> dye lasers,<sup>5</sup> in manufacture of vinyl polymers,<sup>6</sup> textiles<sup>1</sup> determination of iron,<sup>7</sup> calcium,<sup>8</sup> aluminum,<sup>9–11</sup> tantalum,<sup>12</sup> monitoring hardness in industrial water,<sup>13</sup> measuring chlorine dioxide in drinking water,<sup>14</sup> hypoglycemic agents,<sup>15</sup> nuclear fluorochrome<sup>16</sup>

**Safety/Toxicity** Mutagenicity<sup>17</sup>

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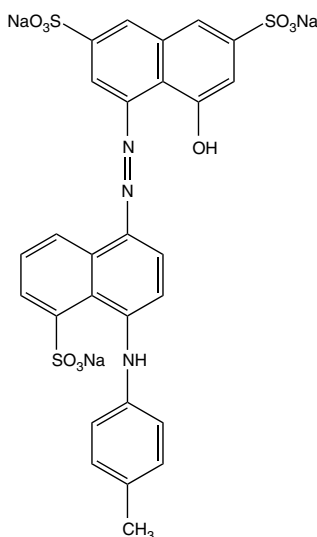
**ACID BLUE 89**

**Other Names** C.I. Acid Blue 89, trisodium salt; Acid Blue Sh; Acid Light Blue; Acid Sky Blue; Acilan Fast Navy Blue B; Atul Acid Sulfon Blue B; C.I. 13405; C.I. Acid Blue 89; Calcocid Wool Blue B; Cirene Brilliant Blue B; Eniacid Brilliant Blue B; Fast Wool Blue B; Hispacid Fast Blue B; Russian Acid Blue; Sulfonine Acid Blue B; Sulphon Acid Blue B; Tertracid Fast Flue SB

**CA Index Name** 2,7-Naphthalenedisulfonic acid, 4-hydroxy-5-[[4-[(4-methylphenyl)amino]-5-sulfo-1-naphthalenyl]azo]-, trisodium salt

**CAS Registry Number** 10359-95-2

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>27</sub>H<sub>18</sub>N<sub>3</sub>O<sub>10</sub>S<sub>3</sub>Na<sub>3</sub>

**Molecular Weight** 709.61

**pH Range** 11.0–12.0

**Color Change at pH** Blue (11.0) to red (12.0)

**pKa** 11.29

**Physical Form** Brown powder

**Solubility** Soluble in water, ethanol

**Melting Point** >250°C

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Wool dyeing,<sup>2</sup> tints for polyester fibers,<sup>3</sup> coloring metal oxide<sup>4</sup>

**Safety/Toxicity** No data available

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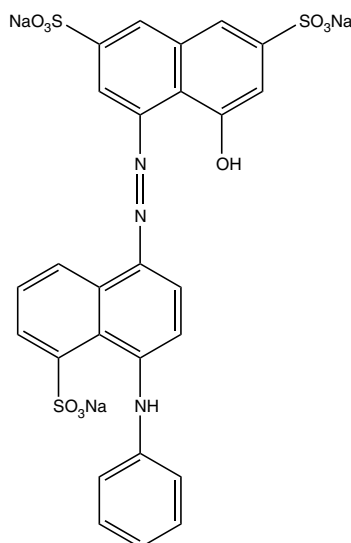
## ACID BLUE 92

**Other Names** Acid Blue 2K; C.I. Acid Blue 92; C.I. Acid Blue 92, trisodium salt; 4-[(4-Anilino-5-sulfo-1-naphthyl)azo]-5-hydroxy-2,7-naphthalenedisulfonic acid trisodium salt; Acid Blue 92; Acid Blue A; Acid Fast Blue R; Acid Leather Blue R; Acid Wool Blue RL; Acilan Fast Navy Blue R; Airedale Blue RL; Amacid Fast Blue R; Anazolene sodium; Benzyl Blue R; Benzyl Fast Blue R; Best Acid Blue 3R; Bucacid Fast Wool Blue R; C.I. 13390; C.I. Solvent Blue 37; Calcocid Fast Blue SR; Caracid Cyanine Blue R Conc PDR; Cirene Brilliant Blue R; Colacid Blue A; Coomassie Blue Medicinal; Coomassie Blue RL; Cyanine Acid Blue R; Cyanine Acid Blue R New; Fast Acid Blue RL; Fast Wool Blue R; Fenazo Blue SR; Hispacid Fast Blue R; Kayanol Navy Blue R; Lampronol Blue BR; Luxol Fast Blue AR; Luxol Fast Blue ARN; Medium Blue EMBL; Methasol Blue RL; Methasol Blue RLX; Pontacyl Fast Blue R; Sepisol Fast Blue ARNF; Sodium anazolene; Solvent Blue 37; Sulfonine Acid Blue R; Sulphon Acid Blue R; Sulphon Acid Blue RA; Sulphon Acid Blue RA Extra; Suminol Fast Navy Blue R; Tertracid Fast Blue SR; Trisodium 4'-anilino-8-hydroxy-1,1'-azonaphthalene-3,6,5'-trisulfonate; Vondamol Fast Blue R; Wool Blue RL; Wool Fast Blue R

**CA Index Name** 2,7-Naphthalenedisulfonic acid, 4-hydroxy-5-[[4-(phenylamino)-5-sulfo-1-naphthalenyl]azo]-, trisodium salt

**CAS Registry Number** 3861-73-2

**Merck Index Number** 628

**Chemical Structure**

**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{26}H_{16}N_3O_{10}S_3Na_3$

**Molecular Weight** 695.59

**pH Range** 11.0–12.0

**Color Change at pH** Blue (11.0) to pink (12.0)

**pKa** 11.22

**Physical Form** Dark bluish-black powder

**Solubility** Soluble in water, acetone; slightly soluble in ethanol, glycerol

**UV-Visible** ( $\lambda_{max}$ ) 571 nm, 585 nm, 580–590 nm

**Melting Point** >300°C

**Synthesis** Synthetic methods<sup>1–6</sup>

**Major Applications** Color filter,<sup>7,8</sup> fuel cells,<sup>9</sup> thin films,<sup>1</sup> inks,<sup>10</sup> markers,<sup>11</sup> lithographic printing plates,<sup>12</sup> textiles,<sup>13</sup> cosmetics,<sup>14</sup> neural network<sup>15</sup>

**Safety/Toxicity** Genotoxicity<sup>16</sup>

**A**

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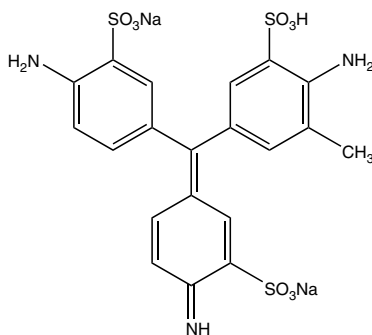
## ACID FUCHSIN

**Other Names** C.I. Acid Violet 19; C.I. Acid Violet 19, disodium salt; Rubine S; Acid Fuchsin; Acid Fuchsin FB; Acid Fuchsin N; Acid Fuchsin O; Acid Fuchsin S; Acid Leather Magenta A; Acid Magenta; Acid Magenta O; Acid Violet 19; Acid fuchsin sodium salt; Acid rosein; Acid rubin; Acidal Fuchsin; Acidal Magenta; C.I. 42685; Fuchsin S; Fuchsin acid; Fuchsin acid; Kiton Magenta A; *p*-Fuchsin acid

**CA Index Name** Benzenesulfonic acid, 2-amino-5-[(4-amino-3-sulphophenyl)(4-imino-3-sulfo-2,5-cyclohexadien-1-ylidene)methyl]-3-methyl-, disodium salt

**CAS Registry Number** 3244-88-0

**Merck Index Number** 107

**Chemical Structure**

**Chemical/Dye Class** Triphenylmethane

**Molecular Formula**  $C_{20}H_{17}N_3O_9S_3Na_2$

**Molecular Weight** 585.55

**pH Range** 12.0–14.0

**Color Change at pH** Red (12.0) to colorless (14.0)

**Physical Form** Dark green crystals

**Solubility** Very soluble in water; slightly soluble to insoluble in ethanol; insoluble in xylene

**UV-Visible** ( $\lambda_{max}$ ) 546 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Nanocomposite,<sup>3</sup> recording materials,<sup>4</sup> sol-gel matrix,<sup>5</sup> decoder system,<sup>6</sup> color filter,<sup>7</sup> inks,<sup>8</sup> paints,<sup>9</sup> markers,<sup>10</sup> highlighters,<sup>11</sup> corrosion inhibitors,<sup>12</sup> explosives,<sup>13</sup> packaging system,<sup>14</sup> textiles,<sup>15</sup> hair dyes,<sup>16</sup> make-up,<sup>17</sup> cosmetics,<sup>18</sup> food storage,<sup>19</sup> dental bleaching,<sup>20</sup> detecting tumor cells,<sup>21</sup> determine bacterial growth,<sup>22</sup> cancer chemopreventive activity<sup>23</sup>

**Safety/Toxicity** Genotoxicity,<sup>24</sup> oral toxicity,<sup>25</sup> neurotoxicity<sup>26</sup>

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## ACRIDINE

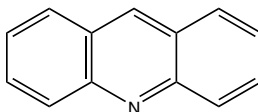
**Other Names** 10-Azaanthracene; 2,3-Benzoquinoline; 9-Azaanthracene; Benzo[b]quinoline; Dibenzo[b,e]pyridine; NSC 3408

**CA Index Name** Acridine

**CAS Registry Number** 260-94-6

**Merck Index Number** 122

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Acridine

**Molecular Formula** C<sub>13</sub>H<sub>9</sub>N

**Molecular Weight:** 179.22

**pH Range:** 5.2–6.6

**Color Change at pH:** Green fluorescence (5.2) to violet fluorescence (6.6)

**pKa** 5.50

**Physical Form** Yellow powder

**Solubility** Slightly soluble in boiling water; freely soluble in ethanol, ether

**UV-Visible** ( $\lambda_{\max}$ ) 358 nm, 392 nm

**Melting Point:** 107–111°C

**Boiling Point** 346°C

**Synthesis** Synthetic methods<sup>1–13</sup>

**Major Applications** Organic light-emitting diode,<sup>14</sup> photoresists,<sup>15</sup> nanosensors,<sup>16</sup> fuel cells,<sup>17</sup> memory device,<sup>18</sup> semiconductors,<sup>19</sup> information storage device,<sup>20</sup> liquid crystal displays,<sup>21</sup> identification of product forgeries,<sup>22</sup> inks,<sup>23</sup> adhesives,<sup>23</sup> textile,<sup>24</sup> hair dyes,<sup>25</sup> gene detection assay,<sup>26</sup> staining cells,<sup>27</sup> biosensors,<sup>28</sup> detecting nucleic acids,<sup>29</sup> proteins,<sup>29</sup> anti-HCV antibodies,<sup>30</sup> antibacterial,<sup>31</sup> anti-amyloid agents,<sup>32</sup> wound dressing materials,<sup>33</sup> vaccines against infection,<sup>34</sup> allergy<sup>34</sup> and cancer<sup>34</sup>

**Safety/Toxicity** Acute toxicity,<sup>35</sup> bacterial toxicity,<sup>36</sup> carcinogenicity,<sup>37</sup> chronic toxicity,<sup>38</sup> cytotoxicity,<sup>39</sup> ecotoxicity,<sup>40</sup> genotoxicity,<sup>41</sup> mutagenicity,<sup>42</sup> phototoxicity,<sup>43</sup> phytotoxicity<sup>44</sup>

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## ALIZARIN RED

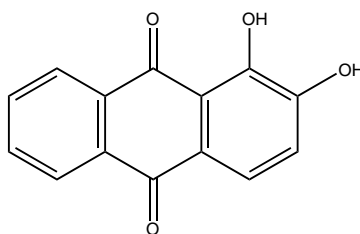
**Other Names** Alizarin B; Anthraquinone, 1,2-dihydroxy-; 1,2-Anthraquinonediol; 1,2-Dihydroxy-9,10-anthracenedione; 1,2-Dihydroxy-9,10-anthraquinone; 1,2-Dihydroxyanthraquinone; Acid Metachrome Red B; Acid Mordant Red B; Alizarin; Alizarin Red; Alizarina; Alizarine; Alizarine 3B; Alizarine B; Alizarine Indicator; Alizarine L Paste; Alizarine Lake Red 2P; Alizarine Lake Red 3P; Alizarine Lake Red IPX; Alizarine NAC; Alizarine Paste 20 percent Bluish; Alizarine Red; Alizarine Red B; Alizarine Red B2; Alizarine Red IP; Alizarine Red IPP; Alizarine Red L; C Ext. Red 62; C.I. 58000; C.I. Mordant Red 11; Certiqua Alizarine; D And C Orange Number 15; Deep Crimson Madder 10821; Eljon Madder; Mitsui Alizarine B; Mordant Red 11; NSC 7212; Turkey Red

**CA Index Name** 9,10-Anthracenedione, 1,2-dihydroxy-

**CAS Registry Number** 72-48-0

**Merck Index Number** 251

**Chemical Structure**



**Chemical/Dye Class** Miscellaneous, Anthraquinone

**Molecular Formula** C<sub>14</sub>H<sub>8</sub>O<sub>4</sub>

**Molecular Weight** 240.21

**pH Range** 5.5–6.8;

10.1–12.1

**Color Change at pH** Yellow (5.5) to red (6.8)

Red (10.1) to purple (12.1)

**pKa** 6.77

**Physical Form** Orange powder

**Solubility** Virtually insoluble in water; moderately soluble in ethanol, soluble in benzene, toluene, xylene, pyridine, acetic acid

**UV-Visible (λ<sub>max</sub>)** 567 nm, 609 nm

**Melting Point** 290°C

**Boiling Point** 430°C

**Synthesis** Synthetic methods<sup>1–8</sup>

**Major Applications** Plasma displays,<sup>9</sup> antireflective coatings,<sup>10</sup> chemical-mechanical polishing,<sup>11</sup> photoreceptors,<sup>12</sup> glass coatings,<sup>13</sup> paints,<sup>14</sup> anticorrosion coatings,<sup>15</sup> thermoplastics,<sup>16</sup> wood coloring,<sup>17</sup> textiles,<sup>18</sup> pH sensor device,<sup>19</sup> detergent,<sup>20</sup> hair dyes,<sup>21</sup> darkening skin,<sup>22</sup> cosmetics,<sup>23</sup> parasiticide,<sup>24</sup> antifungal agent<sup>25</sup>

**Safety/Toxicity** Acute and subacute toxicity,<sup>26</sup> carcinogenicity,<sup>27</sup> environmental contaminants,<sup>28</sup> estrogenicity,<sup>29</sup> genotoxicity,<sup>30</sup> hypersensitivity,<sup>31</sup> mutagenicity,<sup>32</sup> photoinduced toxicity,<sup>33</sup> synergistic toxicity<sup>34</sup>

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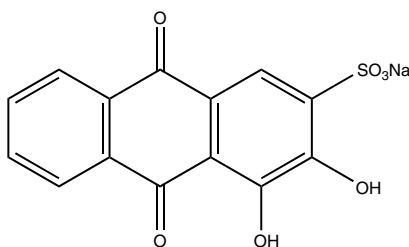
## ALIZARIN RED S

**Other Names** 2-Anthraquinonesulfonic acid, 3,4-dihydroxy-, sodium salt; Acid Mordant Red SW; Acid Red Alizarine; Ahcoquinone Red S; Alizarin Carmine; Alizarin Red S; Alizarin S; Alizarine Carmine; Alizarine Carmine Indicator; Alizarine Red A; Alizarine Red AS; Alizarine Red Indicator; Alizarine Red S; Alizarine Red S sodium salt; Alizarine Red SW; Alizarine Red SZ; Alizarine Red W; Alizarine Red WA; Alizarine Red WS; Alizarine Red for Wool; Alizarine S; Alizarine S Extra Conc. A Export; Alizarine S Extra Pure A; Alizarinsulfonate; C.I. 58005; C.I. Mordant Red 3; Calcochrome Alizarine Red SC; Carnelio Rubine Lake; Chrome Red Alizarine; Diamond Red W; Ext D and C Red No. 7; Fenakrom Red W; Mitsui Alizarine Red S; Mordant Red 3; Oxanal Fast Red SW; Sodium 3,4-dihydroxyanthraquinone-2-sulfonate; Sodium alizarin-3-sulfonate; Sodium alizarinesulfonate; Sodium alizarinsulfonate

**CA Index Name** 2-Anthracenesulfonic acid, 9,10-dihydro-3,4-dihydroxy-9,10-dioxo-, monosodium salt

**CAS Registry Number** 130-22-3

**Merck Index Number** 8573

**Chemical Structure**

**Chemical/Dye Class** Anthraquinone

**Molecular Formula**  $C_{14}H_7O_7SNa$

**Molecular Weight** 342.26

**pH Range** 3.5–6.5;

9.4–12.0

**Color Change at pH** Yellow (3.5) to red (6.5)

Orange (9.4) to violet (12.0)

**pKa** 4.5, 11

**Physical Form** Orange-yellow powder

**Solubility** Freely soluble in water; soluble in ethanol; insoluble in ether

**UV-Visible** ( $\lambda_{max}$ ) 556 nm, 596 nm, 423 nm, 546 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Nanocomposite material,<sup>6</sup> chemical mechanical polishing,<sup>7</sup> optical fibers,<sup>8</sup> display device,<sup>9</sup> carbon nanotubes,<sup>10</sup> textiles,<sup>11</sup> determination of aluminum,<sup>12</sup> iron,<sup>12</sup> copper,<sup>12</sup> manganese,<sup>13</sup> zinc,<sup>13</sup> calcium,<sup>14</sup> magnesium,<sup>14</sup> zirconium,<sup>15</sup> hafnium,<sup>15</sup> molybdenum,<sup>16</sup> uranium,<sup>17</sup> vanadium,<sup>18</sup> detergents,<sup>19</sup> hair dyes,<sup>20</sup> determination of proteins,<sup>21</sup> clotrimazole,<sup>22</sup> ketoconazole,<sup>22</sup> piroxicam, and tenoxicam<sup>23</sup>

**Safety/Toxicity** Carcinogenicity,<sup>24</sup> cytotoxicity,<sup>25</sup> genotoxicity,<sup>25</sup> toxicity to freshwater organisms,<sup>26</sup> environmental and pollutants<sup>27</sup>

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## A

## ALIZARIN YELLOW GG

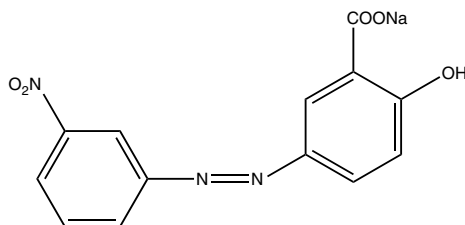
**Other Names** C.I. Mordant Yellow 1; C.I. Mordant Yellow 1, monosodium salt; Salicylic acid, 5-(*m*-nitrophenylazo)-, sodium salt; Acid Chrome Yellow 2GW; Acid Chrome Yellow GG; Alizarin Yellow; Alizarin Yellow G; Alizarin Yellow G sodium salt; Alizarin Yellow GG; Alizarine Yellow 2G; Alizarine Yellow AGP; Alizarine Yellow G; Alizarine Yellow GG; Alizarine Yellow GGW; Alizarine Yellow GM; Alizarine Yellow GR; Alizarol Yellow GW; Anthranol Chrome Yellow 2G; Anthranol Chrome Yellow 5GS; Atlantichrome Yellow 2G; Azochromol Yellow 5G; C.I. 14025; Calcochrome Yellow 2G; Chrome Fast Yellow RW; Chrome Yellow 2G; Chrome Yellow 2GR; Chromol Yellow G; Chromol Yellow N; Cromal Yellow M; Eniacromo Yellow G; Eriochromal Yellow 2G; Eriochrome Yellow 2G; Eriochrome Yellow GS; Fenakrom Yellow R; Hidachrome Yellow 2G; Hispacrom Yellow 2G; Hispacrom Yellow 2GR; Java Chrome Yellow GT; Java Unichrome Yellow GT; Kayaku Mordant Yellow GG; Magracrom Yellow GG; Metachrome Yellow; Metachrome Yellow RA; Metomega Chrome Yellow GM; Mitsui Chrome Yellow GG; Monochrome Yellow MG; Orthochrome Yellow GGW; Pontachrome Yellow GS; RV 1; Salicyl yellow; Salicylic acid, (*m*-nitrophenylazo)-, sodium salt; Showa Chrome Yellow GG; Sodium 5-(*m*-nitrophenylazo) salicylate; Sodium 5-[(3-nitrophenyl)-azo]-salicylate; Sodium *m*-nitrobenzeneazosalicylate; Solochrome Yellow WN; Sunchromine Yellow GG; Yodochrome Yellow GGN

**CA Index Name** Benzoic acid, 2-hydroxy-5-[(3-nitrophenyl)azo]-, monosodium salt

**CAS Registry Number** 584-42-9

**Merck Index Number** 5919

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{13}H_8N_3O_5Na$

**Molecular Weight** 309.22

**pH Range** 10.0–12.0

**Color Change at pH** Yellow (10.0) to orange (12.0)

**Physical Form** Yellow-orange powder

**Solubility** Soluble in water, methyl cellosolve; slightly soluble in ethanol, acetone

**UV-Visible** ( $\lambda_{max}$ ) 362 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1-3</sup>

**Major Applications** Optical engineering applications,<sup>4</sup> sensors,<sup>5</sup> making masks,<sup>6</sup> electrorheological materials,<sup>7</sup> surface treatment of copper,<sup>8</sup> coloring zinc,<sup>9</sup> aluminum,<sup>10</sup> corrosion testing,<sup>11</sup> adhesive,<sup>12</sup> lubricants,<sup>13</sup> textiles,<sup>14</sup> food storage,<sup>15</sup> determine bacterial growth,<sup>16</sup> pharmaceutical preparations<sup>17</sup>

**Safety/Toxicity** Mutagenicity<sup>18</sup>

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## A

## ALIZARIN YELLOW R

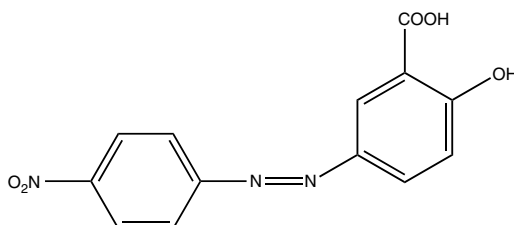
**Other Names** C.I. Mordant Orange 1; Salicylic acid, 5-(*p*-nitrophenylazo)-; 2-Hydroxy-5-(4-nitrophenylazo)benzoic acid; 4-Nitrobenzene-1-azo-5-salicylic acid; 5-(4-Nitrophenylazo)salicylic acid; Acid Alizarine Yellow R; Alizarin Yellow R; Alizarin orange; Alizarine Chrome Orange G; Alizarine Orange 2GN; Alizarine Orange R; Alizarine Orange RD; Alizarine Yellow P; Alizarine Yellow R; Alizarine Yellow R-CF; Alizarol Orange R; Alphacroic Orange R; Anthranol Chrome Yellow R; Azochromol Orange R; Brasilan Chrome Orange R; C.I. 14030; Calcochrome Orange R; Chromacid Orange S; Chrome Fast Orange RW; Chrome Orange; Chrome Orange MR; Chrome Orange N; Chrome Orange R; Chrome Orange RLE; Chrome Yellow 3RN; Chromol Orange R extra; Diamond Chrome Yellow 3R; Durochrome Yellow 2RN; Eniacromo Orange R; Eriochrome Orange AOR; Fenakrom Orange R; Hidachrome Orange R; Hispacrom Orange R; Java Chrome Yellow 3R; Java Unichrome Yellow 3R; KCA Chrome Orange R; Kenachrome Orange; Lighthouse Chrome Orange; Magracrom orange; Metachrome Orange R; Mitsui Chrome Orange A; Mitsui Chrome Orange AN; Monochrome Orange R; Monochrome Yellow 3R; Mordant Orange 1; Orthochrome Orange R; PNBAS; Peerachrome Yellow R; Pontachrome Yellow 3RN; RV 2; Solochrome Orange M; Synchromate Orange AOR; Terra Cotta RRN; Terracotta 2RN; Tertrochrome Yellow 3R; Yodochrome Orange A; *p*-Nitrobenzeneazosalicilyc acid

**CA Index Name** Benzoic acid, 2-hydroxy-5-[(4-nitrophenyl)azo]-

**CAS Registry Number** 2243-76-7

**Merck Index Number** 255

**Chemical Structure**



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>13</sub>H<sub>9</sub>N<sub>3</sub>O<sub>5</sub>

**Molecular Weight** 287.23

**pH Range** 10.0–12.1

**Color Change at pH** Yellow (10.0) to orange-red (12.1)

**pKa** 2.85

**Physical Form** Orange-brown powder

**Solubility** Soluble in water, ethanol; slightly soluble in acetone

**UV-Visible** ( $\lambda_{\text{max}}$ ) 385 nm

**Melting Point** 253–254°C (decompose)

**Boiling Point (Calcd.)** 571.4 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1-4</sup>

**Major Applications** Display device,<sup>5</sup> photoresist,<sup>6</sup> nanoparticles,<sup>7</sup> sensors,<sup>8,9</sup> image-recoring materials,<sup>10</sup> photoconductive materials,<sup>11,12</sup> photography,<sup>13</sup> electrorheological materials,<sup>14</sup> copying materials,<sup>15</sup> optical engineering applications,<sup>16</sup> monitoring oil degradation,<sup>17</sup> lubricant,<sup>18</sup> flame luminosity enhancing agent,<sup>19</sup> coloring zinc,<sup>20</sup> method for polymerization of vinyl chloride,<sup>21</sup> determination of OH groups on resins,<sup>22</sup> cosmetics,<sup>23</sup> diapers,<sup>24</sup> food storage,<sup>25</sup> measurement of acidity in juice,<sup>26</sup> assay for aldehyde contents,<sup>27</sup> determination of albumin,<sup>28</sup> agent for plaque,<sup>29</sup> method for counting leukocytes,<sup>30</sup> antifungal agent<sup>31</sup>

**Safety/Toxicity** Toxicity,<sup>32</sup> mutagenicity<sup>33</sup>

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## ALKALI BLUE

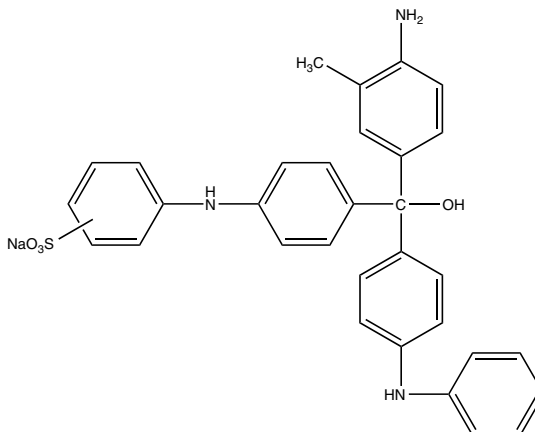
**Other Names** Alkali Blue 6B; Acid Blue 110

**CA Index Name** Benzenesulfonic acid, [[4-[(4-amino-3-methylphenyl)hydroxy[4-(phenylamino)phenyl]methyl]phenyl]amino]-, monosodium salt

**CAS Registry Number** 30586-13-1

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Triphenylmethane

**Molecular Formula** C<sub>32</sub>H<sub>28</sub>N<sub>3</sub>O<sub>4</sub>SNa

**Molecular Weight** 573.65

**pH Range** 9.4–14.0

**Color Change at pH** Blue-violet (9.4) to red-pink (14.0)

**Physical Form** Dark blue powder

**Solubility** Sparingly soluble in water; soluble in ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 603 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1</sup>

**Major Applications** Electrostatographic dry developers,<sup>1</sup> chelators for iron overload<sup>2</sup>

**Safety/Toxicity** No data available

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## 9-AMINO-6-CHLORO-2-METHOXYACRIDINE

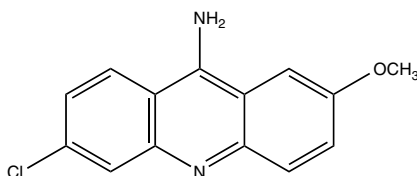
**Other Names** Acridine, 9-amino-6-chloro-2-methoxy-; 2-Methoxy-6-chloro-9-aminoacridine; 3-Chloro-7-methoxy-9-aminoacridine; 6-Chloro-9-amino-2-methoxyacridine; 9-Amino-3-chloro-7-methoxyacridine; 9-Amino-6-chloro-2-methoxyacridine; G 185; NSC 15300

**CA Index Name** 9-Acridinamine, 6-chloro-2-methoxy-

**CAS Registry Number** 3548-09-2

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>14</sub>H<sub>11</sub>ClN<sub>2</sub>O

**Molecular Weight** 258.70

**pH Range** 7.5–9.8

**Color Change at pH** Weak blue fluorescence (7.5) to strong blue fluorescence (9.8)

**pKa** 8.6

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in *N,N*-dimethylformamide, dimethyl sulfoxide

**UV-Visible** ( $\lambda_{\text{max}}$ ) 412 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 475.1 ± 35.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–7</sup>

**Major Applications** Sensors,<sup>8</sup> detection method for DNA amplification,<sup>9</sup> inhibition of neurodegenerative diseases,<sup>10</sup> RNA hydrolysis,<sup>11,12</sup> fluorescent probes,<sup>13,14</sup> primers for nucleic acid sequencing,<sup>15</sup> synthesis of nucleic acids,<sup>16</sup> antimalarial agent<sup>17</sup>

**Safety/Toxicity** Genotoxicity,<sup>18</sup> mutagenicity<sup>19–21</sup>

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## 5-AMINOSALICYLIC ACID

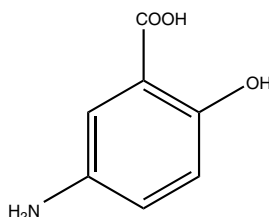
**Other Names** Salicylic acid, 5-amino-; 2-Hydroxy-5-aminobenzoic acid; 3-Carboxy-4-hydroxy-aniline; 5-ASA; 5-Amino-2-hydroxybenzoic acid; 5-Aminosalicylic acid; Asacol; Asacolitin; Asacolon; Canasa; Claversal; Fisalamine; Ipocol; Lixacol; Mesacol; Mesalamine; Mesalazine; Mesasal; NSC 38877; Pentasa; Rowasa; Salofalk; Salozinal; *m*-Aminosalicylic acid

**CA Index Name** Benzoic acid, 5-amino-2-hydroxy-

**CAS Registry Number** 89-57-6

**Merck Index Number** 5904

**Chemical Structure**



**Chemical/Dye Class** Fluorescent

**Molecular Formula**  $C_7H_7NO_3$

**Molecular Weight** 153.14

**pH Range** 3.1–4.4

**Color Change at pH** Non-fluorescence (3.1) to light green fluorescence (4.4)

**pKa** 2.74, 5.84

**Physical Form** White to pinkish crystals

**Solubility** Slightly soluble in cold water, ethanol; more soluble in hot water; soluble in hydrochloric acid

**Melting Point** 280°C (decompose)

**Boiling Point (Calcd.)** 403.9 ± 40.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–14</sup>

**Major Applications** Detergent,<sup>15</sup> hair dyes,<sup>16</sup> prevention of colorectal cancer,<sup>17</sup> treating inflammatory bowel disease,<sup>18</sup> autoimmune disorders,<sup>19</sup> gastrointestinal inflammation,<sup>20</sup> chemokine-mediated diseases,<sup>21</sup> mucosal tissue disorder,<sup>22</sup> sleep disorders,<sup>23</sup> rectoanal tenesmus,<sup>24</sup> ulcerative colitis<sup>25</sup>

**Safety/Toxicity** Hepatotoxicity,<sup>26,27</sup> cytotoxicity,<sup>27,28</sup> nephrotoxicity,<sup>29</sup> risk of renal disease,<sup>30</sup> safety in pregnancy,<sup>31</sup> side effects<sup>32</sup>

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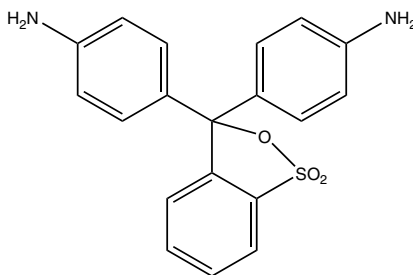
## ANILINESULFONEPHTHALEIN

**Other Names** Aniline, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)di-, S,S-dioxide; Benzenamine, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)*bis*-, S,S-dioxide; *o*-Toluenesulfonic acid,  $\alpha,\alpha$ -*bis*(*p*-aminophenyl)- $\alpha$ -hydroxy-,  $\gamma$ -sultone; 3H-2,1-Benzoxathiole, benzenamine deriv.; Anilinesulfonephthalein

**CA Index Name** Benzenamine, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*-

**CAS Registry Number** 4538-11-8

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>19</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>S

**Molecular Weight** 352.41

**pH Range** 1.32–1.92

11.75–12.53

**Color Change at pH** Yellow (1.32) to violet (1.92)

Violet (11.75) to yellow (12.53)

**pKa** 1.59, 12.26

**Physical Form** Leaflets with green lustre

**Solubility** Soluble in water, ethanol

**Melting Point** >250°C

**Boiling Point (Calcd.)** 570.4 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Phototranschromic materials<sup>2</sup>

**Safety/Toxicity** No data available

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## ANTHRANILIC ACID

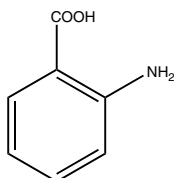
**Other Names** Anthranilic acid;  $\alpha$ -Aminobenzoic acid; 1-Aminobenzene-2-carboxylic acid; 2-Aminobenzoic acid; 2-Carboxyaniline; 2-Carboxyphenylamine; NSC 144; NSC 40929; Vitamin L1; *o*-Aminobenzoic acid; *o*-Anthranilic acid; *o*-Carboxyaniline

**CA Index Name** Benzoic acid, 2-amino-

**CAS Registry Number** 118-92-3

**Merck Index Number** 422

**Chemical Structure**



**Chemical/Dye Class** Fluorescent

**Molecular Formula**  $C_7H_7NO_2$

**Molecular Weight** 137.14

**pH Range** 1.5–3.0

4.5–6.0

12.5–14.0

**Color Change at pH** Non-fluorescence (1.5) light blue fluorescence (3.0)

Light blue fluorescence (4.5) to dark blue fluorescence (6.0)

Dark blue fluorescence (12.5) to non-fluorescence (14.0)

**pKa** 1.85, 4.95

**Physical Form** White to pale yellow crystalline powder

**Solubility** Sparingly soluble in cold water; freely soluble in hot water, ethanol, ether

**Melting Point** 144–147°C

**Boiling Point (Calcd.)**  $311.9 \pm 25.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Bottom antireflective coatings,<sup>6</sup> semiconductor devices,<sup>7</sup> inks,<sup>8</sup> hair dyes,<sup>9</sup> cosmetics,<sup>10,11</sup> treatment of chronic inflammatory diseases,<sup>12</sup> depression<sup>13</sup>

**Safety/Toxicity** Acute oral toxicity,<sup>14</sup> carcinogenicity,<sup>15</sup> ecotoxicity,<sup>16</sup> genotoxicity,<sup>17</sup> mutagenicity,<sup>18</sup> neurotoxicity,<sup>19</sup> tumorigenicity<sup>20</sup>

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## AURIN

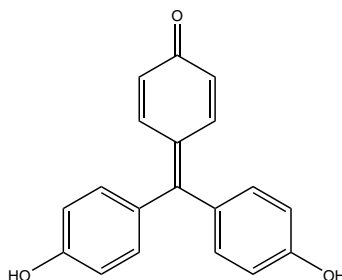
**Other Names** 2,5-Cyclohexadien-1-one, 4-[*bis*(*p*-hydroxyphenyl)methylene]-; Aurin; 4,4'-Dihydroxyfuchson; 4-(*p,p'*-Dihydroxybenzhydridene)-2,5-cyclohexadien-1-one; 4-[*Bis*(*p*-hydroxyphenyl)methylene]-2,5-cyclohexadien-1-one; Aurin 555; Aurine; C.I. 43800; Corallin; Corallin Spirit Soluble; NSC 7805; Pararosolic acid; Rosalic acid; Spirit Aurine; *p*-Rosolic acid

**CA Index Name** 2,5-Cyclohexadien-1-one, 4-[*bis*(4-hydroxyphenyl)methylene]-

**CAS Registry Number** 603-45-2

**Merck Index Number** 881

**Chemical Structure**



**Chemical/Dye Class** Triphenylmethane

**Molecular Formula** C<sub>19</sub>H<sub>14</sub>O<sub>3</sub>

**Molecular Weight** 290.31

**pH Range** 6.6–8.0

**Color Change at pH** Yellow (6.6) to red (8.0)

**pKa** 6.98

**Physical Form** Red crystals

**Solubility** Practically insoluble in water, benzene; freely soluble in ethanol

**UV-Visible** (λ<sub>max</sub>) 534.6 nm, 479.5 nm, 482 nm

**Melting Point** 309°C (decompose)

**Boiling Point (Calcd.)** 543.0 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–9</sup>

**Major Applications** Antireflective coatings,<sup>10</sup> thermochromic materials,<sup>11</sup> photoresists,<sup>2</sup> electrorheological materials,<sup>12</sup> film patterning,<sup>13</sup> recording materials,<sup>14</sup> lithium battery,<sup>15</sup> semiconductors,<sup>16</sup> printing materials,<sup>17</sup> inks,<sup>18</sup> corrosion inhibitors,<sup>19</sup> adhesives,<sup>20</sup> drugs,<sup>21</sup> detecting viable cells,<sup>22</sup> treatment of Alzheimer's disease<sup>1</sup>

**Safety/Toxicity** Toxic activity,<sup>23</sup> environmental toxicity,<sup>24</sup> cytopathogenicity<sup>25</sup>

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# B

## BENZAURIN

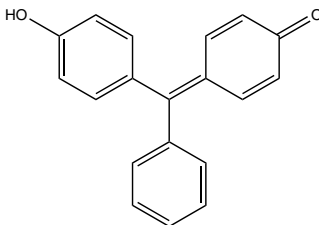
**Other Names** 2,5-Cyclohexadien-1-one, 4-(*p*-hydroxy- $\alpha$ -phenylbenzylidene)-; Benzaurin; NSC 55861; Phenolbenzein; Rosolic acid

**CA Index Name** 2,5-Cyclohexadien-1-one, 4-[(4-hydroxyphenyl)phenylmethylene]-

**CAS Registry Number** 569-60-8

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Benzein

**Molecular Formula** C<sub>19</sub>H<sub>14</sub>O<sub>2</sub>

**Molecular Weight** 274.31

**pH Range** 6.0–7.6

**Color Change at pH** Yellow (6.0) to red (7.6)

**pKa** 9.28

**Physical Form** Orange-red crystals

**Solubility** Insoluble in water; soluble in ethanol

**Melting Point** >250°C

**Boiling Point (Calcd.)** 497.0 ± 45.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Indicator<sup>6</sup>

**Safety/Toxicity** No data available

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## BENZOPURPURIN 4B

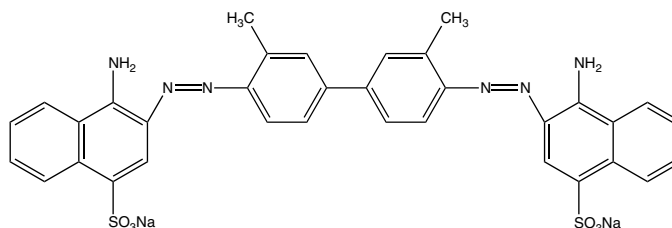
**Other Names** C.I. Direct Red 2; C.I. Direct Red 2, disodium salt; Amanil Purpurine 4B; Atul Direct Red 4B; Azamin 4B; Azocard Red 4B; Bencidal Purple 4B; Benzanil Purpurine 4B; Benzopurpurin 4B; Benzopurpurin B; Benzopurpurine 4B; Benzopurpurine 4BKX; Benzopurpurine 4BX; Brasilamina Red 4B; C.I. 23500; Calcomine Red 4BX; Chrome Leather Red 4B; Cotton Red 4B; Diacotton Benzopurpurine 4B; Diamine Purpurine 4B; Diaphtamine Purpurine 4B; Diazamine Purpurine 4B; Diazine Red 4B; Diazol Purpurine 4B; Diphenyl Red 4B; Diphenyl Red 4BS; Direct Purpurine 4B; Direct Purpurine M 4B; Direct Red 2; Direct Red 4A; Direct Red 4B; Direct Red DCB; Eclipse Red; Erie Benzo 4BP; Erie Red 4B; Fast Scarlet; Hispamin Red 4B; Kayaku Benzopurpurine 4B; Mitsui Benzopurpurine 4BX; Paper Red 4BS; Phenamine Purpurine 4B; Purpurin 4By; Purpurine 4B; Red 4B; Sultan 4B; Sultan Red 4B; Tertrodirect Red 4B

**CA Index Name** 1-Naphthalenesulfonic acid, 3,3'-[(3,3'-dimethyl[1,1'-biphenyl]-4,4'-diyl)*bis*(azo)]*bis*[4-amino-, disodium salt

**CAS Registry Number** 992-59-6

**Merck Index Number** 1101

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>34</sub>H<sub>26</sub>N<sub>6</sub>O<sub>6</sub>S<sub>2</sub>Na<sub>2</sub>

**Molecular Weight** 724.73

**pH Range** 1.2–4.0

**Color Change at pH** Blue-violet (1.2) to red (4.0)

**Physical Form** Brown powder

**Solubility** Soluble in water, ethanol, acetone, sodium hydroxide, sulfuric acid

**UV-Visible** (λ<sub>max</sub>) 500 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Liquid crystal displays,<sup>4</sup> thin films,<sup>5</sup> electronic devices,<sup>6</sup> inks,<sup>7</sup> lithographic printing plates,<sup>8</sup> printing and dyeing applications,<sup>9</sup> textiles,<sup>10</sup> lubricants,<sup>11</sup> food storage,<sup>12</sup> microorganism staining agent,<sup>13</sup> treatment of apolipoprotein E-related diseases,<sup>14</sup> antifungal agent<sup>15</sup>

**Safety/Toxicity** Genotoxicity,<sup>16</sup> mutagenicity<sup>17,18</sup>

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## BRILLIANT GREEN

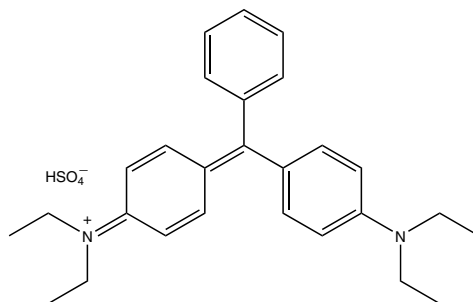
**Other Names** C.I. Basic Green 1; 12415 Green; ADC Brilliant Green Crystals; Aizen Diamond Green GH; Aizen Malachite Green GH; Astra Diamond Green GX; Astrazon Green D; Avon Green A 4379; Basic Bright Green; Basic Bright Green Sulfate; Basic Brilliant Green; Basic Green 1; Basic Green V; Brilliant Green; Brilliant Green B; Brilliant Green BP; Brilliant Green BP Crystals; Brilliant Green BPC; Brilliant Green Crystals; Brilliant Green Crystals H; Brilliant Green DSC; Brilliant Green G; Brilliant Green GX; Brilliant Green Lake; Brilliant Green P; Brilliant Green Special; Brilliant Green Sulfate; Brilliant Green WP Crystals; Brilliant Green Y; Brilliant Green YN; Brilliant Green YNS; Brilliant Lake Green Y; Brilliant green aseptic; C.I. 42040; Calcozine Brilliant Green G; Deorlene Green JJO; Diamond Green G; Diamond Green GH; Ethyl green; Fast Green J; Fast Green JJO; Green EN; Hidaco Brilliant Green; Malachite Green G; Mitsui Brilliant Green GX; NSC 5011; Resplendency Green; Solid Green; Tertrophenne Brilliant Green G; Tokyo Aniline Brilliant Green

**CA Index Name** Ethanaminium, *N*-[4-[[4-(diethylamino)phenyl]phenylmethylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-, sulfate

**CAS Registry Number** 633-03-4

**Merck Index Number** 1374

**Chemical Structure**



**Chemical/Dye Class** Triphenylmethane

**Molecular Formula**  $C_{27}H_{34}N_2O_4S$

**Molecular Weight** 482.63

**pH Range** 0.0–2.6

**Color Change at pH** Yellow (0.0) to green (2.6)

**Physical Form** Green crystals

**Solubility** Soluble in water, ethanol

**UV-Visible** ( $\lambda_{max}$ ) 625 nm, 428 nm

**Melting Point** 210°C (decompose)

**Synthesis** Synthetic methods<sup>1–10</sup>

**Major Applications** Black matrix,<sup>11</sup> color filter,<sup>11</sup> photoresists,<sup>12</sup> sensors,<sup>13</sup> inks,<sup>14</sup> rodenticide,<sup>15</sup> hair dyes,<sup>16</sup> cosmetics,<sup>17</sup> detecting dental carious tissue,<sup>18</sup> *Escherichia coli*,<sup>19</sup> antimalarial agent,<sup>20</sup> wound dressing material,<sup>21</sup> treatment of cancer,<sup>22</sup> medical devices<sup>23</sup>

**Safety/Toxicity** Toxicity to aquatic animals,<sup>24</sup> carcinogenicity<sup>25</sup>

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## BRILLIANT YELLOW

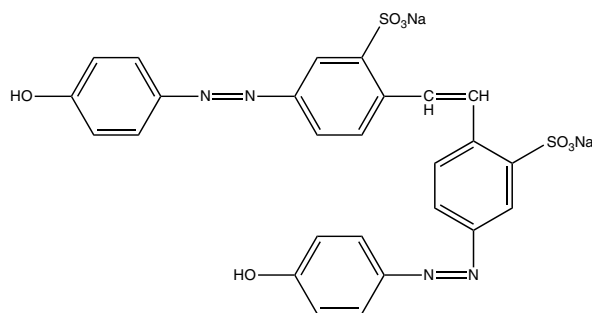
**Other Names** Brilliant Yellow C; C.I. Direct Yellow 4; C.I. Direct Yellow 4, disodium salt; Benzo Brilliant Yellow; Brilliant Fast Yellow G2N; Brilliant Paper Yellow; Brilliant Paper Yellow C; Brilliant Paper Yellow P; Brilliant Yellow; Brilliant Yellow (indicator); C.I. 24890; Calcomine Brilliant Paper Yellow; Chlorazol Brilliant Yellow 3G; Diaphtamine Brilliant Fast Yellow 3G; Diazol Brilliant Yellow N; Direct Brilliant Yellow G; Direct Yellow 4; Fenamin Yellow 3G; Kayaku Direct Yellow G; Nippon Brilliant Yellow G; Paper Yellow 3GX; Paper Yellow 3GXA; Paper Yellow CB; Tertrodirect Yellow B; Trisulfon Paper Yellow

**CA Index Name** Benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-[(4-hydroxyphenyl)azo]-, disodium salt

**CAS Registry Number** 3051-11-4

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{26}H_{18}N_4O_8S_2Na_2$

**Molecular Weight** 624.56

**pH Range** 6.4–8.0

**Color Change at pH** Yellow (6.4) to red-orange (8.0)

**Physical Form** Orange powder

**Solubility** Soluble in water; slightly soluble in ethanol, acetone

**UV-Visible ( $\lambda_{max}$ )** 497 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Display device,<sup>4</sup> sensors,<sup>5,6</sup> photochromic materials,<sup>7</sup> inks,<sup>8</sup> detergent,<sup>9</sup> cosmetics,<sup>10</sup> biosensors,<sup>11</sup> assay for enzyme activity,<sup>12</sup> antifungal agent,<sup>13</sup> antiAIDS agent<sup>14</sup>

**Safety/Toxicity** No data available

### References

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## BROMOCHLOROPHENOL BLUE

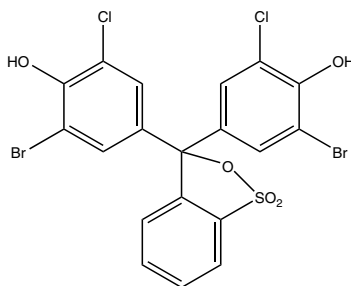
**Other Names** Bromochlorophenol blue; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-chloro-, S,S-dioxide; *o*-Toluenesulfonic acid,  $\alpha,\alpha$ -bis(3-bromo-5-chloro-4-hydroxyphenyl)- $\alpha$ -hydroxy-,  $\gamma$ -sultone; 3H-2,1-Benzoxathiole, phenol deriv.; Bromchlorophenol blue; NSC 7816

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-chloro-

**CAS Registry Number** 2553-71-1

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula**  $C_{19}H_{10}Br_2Cl_2O_5S$

**Molecular Weight** 581.06

**pH Range** 3.0–4.6

**Color Change at pH** Yellow (3.0) to purple (4.6)

**pKa** 6.05

**Physical Form** Violet-pink powder

**Solubility** Sparingly soluble in water; soluble in ethanol

**UV-Visible** ( $\lambda_{max}$ ) 590 nm

**Melting Point** 230°C (decompose)

**Boiling Point (Calcd.)** 602.9  $\pm$  55.0°C Pressure: 760 Torr

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Display device,<sup>2</sup> pH sensors,<sup>3</sup> inks,<sup>4</sup> photoreceptors,<sup>5</sup> lithographic plates,<sup>6</sup> photographic materials,<sup>7</sup> determination of surfactants,<sup>8,9</sup> lubricants,<sup>10</sup> food shelf life,<sup>11,12</sup> in protein assays,<sup>13</sup> vaginal infection test,<sup>14</sup> detecting proteins<sup>15,16</sup>

**Safety/Toxicity** No data available

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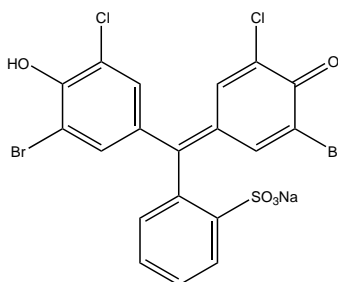
**BROMOCHLOROPHENOL BLUE, SODIUM SALT**

**Other Names** Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-chloro-, S,S-dioxide, monosodium salt; 3H-2,1-Benzoxathiole, phenol deriv.

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-chloro-, monosodium salt

**CAS Registry Number** 102185-52-4

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>19</sub>H<sub>9</sub>Br<sub>2</sub>Cl<sub>2</sub>O<sub>5</sub>SNa

**Molecular Weight** 580.07

**pH Range** 3.0–4.6

**Color Change at pH** Yellow (3.0) to purple (4.6)

**pKa** 6.05

**Physical Form** Black powder

**Solubility** Soluble in water, ethanol

**UV-Visible (λ<sub>max</sub>)** 590 nm

**Melting Point** >250°C

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Chemical probe<sup>2</sup>

**Safety/Toxicity** No data available

**References**

1. Sergeev, G. M.; Korenman, I. M. Composition and stability of complexes of thorium with bromphenol and bromchlorophenol blue. *Zh. Neorg. Khim.* **1978**, 23, 121–125; *Chem. Abstr.* **1978**, 88, 95605.
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## BROMOCRESOL GREEN

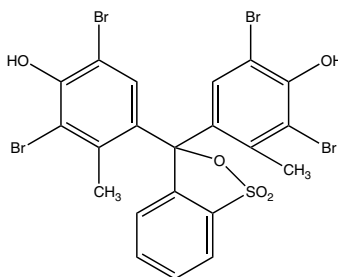
**Other Names** Bromocresol green; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-3-methyl-, S,S-dioxide; *m*-Cresol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-, S,S-dioxide; *o*-Toluenesulfonic acid,  $\alpha,\alpha$ -bis(3,5-dibromo-4-hydroxy-*o*-tolyl)- $\alpha$ -hydroxy-,  $\gamma$ -sultone; 3H-2,1-Benzoxathiole, phenol deriv.; 3',3'',5',5''-Tetrabromo-*m*-cresolsulfonephthalein; BCG; Bromocresol green; NSC 7817; Tetrabromo-*m*-cresolphthalein sulfone

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-3-methyl-

**CAS Registry Number** 76-60-8

**Merck Index Number** 1386

**Chemical Structure**



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>21</sub>H<sub>14</sub>Br<sub>4</sub>O<sub>5</sub>S

**Molecular Weight** 698.01

**pH Range** 3.8–5.4

**Color Change at pH** Yellow (3.8) to blue-green (5.4)

**pKa** 4.7, 4.6

**Physical Form** Slightly yellowish-brownish crystals

**Solubility** Sparingly soluble in water; soluble in ethanol, ether, ethyl acetate

**UV-Visible** ( $\lambda_{\text{max}}$ ) 423 nm, 444 nm, 617 nm

**Melting Point** 218–219°C

**Boiling Point (Calcd.)** 626.0  $\pm$  55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Sol-gel matrix,<sup>4,5</sup> fuel cells,<sup>6</sup> sensors,<sup>7</sup> display device,<sup>8</sup> inks,<sup>9</sup> paints,<sup>10</sup> one-step tester for ammonia,<sup>11</sup> packaging system,<sup>12</sup> textiles,<sup>13</sup> cleansing products,<sup>14</sup> detergents,<sup>15</sup> cosmetics,<sup>16</sup> diapers,<sup>17</sup> identifying fresh and stale rice,<sup>18</sup> monitoring fish spoilage,<sup>19</sup> detecting carbohydrates,<sup>20</sup> lactating acid bacteria,<sup>21</sup> treating neoplasms,<sup>22</sup> cancer,<sup>23</sup> vaginal infection test method,<sup>24</sup> psychoactive drugs,<sup>25</sup> dental materials<sup>26</sup>

**Safety/Toxicity** Effects in the environment,<sup>27</sup> cholestasis,<sup>28</sup> mutagenicity<sup>29</sup>

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**BROMOCRESOL GREEN, SODIUM SALT**

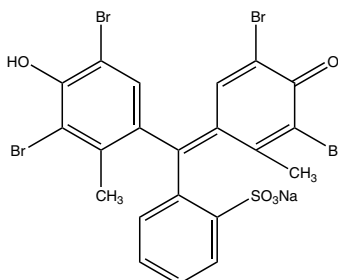
**Other Names** Phenol, 4,4'-(3H-1,2-benzoxathiol-3-ylidene)bis[2,6-dibromo-3-methyl-, S,S-dioxide, monosodium salt; 3H-1,2-Benzoxathiole, phenol deriv.

**CA Index Name** Phenol, 4,4'-(2,2-dioxido-3H-1,2-benzoxathiol-3-ylidene)bis[2,6-dibromo-3-methyl-, monosodium salt

**CAS Registry Number** 62625-32-5

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>21</sub>H<sub>13</sub>Br<sub>4</sub>O<sub>5</sub>Na

**Molecular Weight** 720.02

**pH Range** 3.8–5.4

**Color Change at pH** Yellow (3.8) to blue-green (5.4)

**pKa** 4.6

**Physical Form** Greenish-black crystalline powder

**Solubility** Soluble in water, ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 617 nm, 400 nm

**Melting Point** 230°C (decompose)

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Colloidal pigments<sup>2</sup>

**Safety/Toxicity** No data available

**References**

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## BROMOCRESOL PURPLE

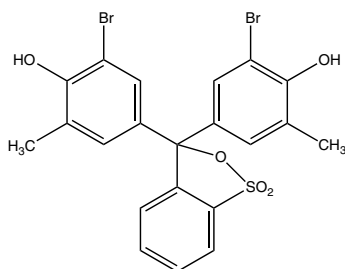
**Other Names** Bromocresol purple; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-methyl-, S,S-dioxide; *o*-Cresol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[6-bromo-, S,S-dioxide; *o*-Toluenesulfonic acid,  $\alpha,\alpha$ -bis(5-bromo-4-hydroxy-*m*-tolyl)- $\alpha$ -hydroxy-,  $\gamma$ -sultone; 3H-2,1-Benzoxathiole, phenol deriv.; Bromcresol purple; NSC 374134

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-methyl-

**CAS Registry Number** 115-40-2

**Merck Index Number** 1387

**Chemical Structure**



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula**  $C_{21}H_{16}Br_2O_5S$

**Molecular Weight** 540.22

**pH Range** 5.2–6.8

**Color Change at pH** Yellow (5.2) to purple (6.8)

**pKa** 6.21, 6.3, 6.4

**Physical Form** Orange-yellow to brick red powder

**Solubility** Sparingly soluble in water; soluble in ethanol, ether, ethyl acetate

**UV-Visible ( $\lambda_{max}$ )** 419 nm, 433 nm, 591 nm

**Melting Point** 241.5°C

**Boiling Point (Calcd.)** 590.2  $\pm$  50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1</sup>

**Major Applications** Waveguides,<sup>2</sup> fuel cells,<sup>3</sup> sensors,<sup>4</sup> sol-gel technology,<sup>5</sup> display device,<sup>6</sup> falsification-proof security paper,<sup>7</sup> paints,<sup>8</sup> detergents,<sup>9</sup> identifying fresh and stale rice,<sup>10</sup> detecting lactic acid bacteria,<sup>11</sup> dental materials,<sup>12</sup> vaginal infection test method<sup>13</sup>

**Safety/Toxicity** Mutagenicity,<sup>14</sup> toxicity<sup>15</sup>

## References

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11. Horikoshi, N.; Okada, Y.; Takeshita, K.; Samejima, T. Semi-solid medium for detecting lactic acid bacteria. Jpn. Kokai Tokkyo Koho JP 2006136272, 2006; *Chem. Abstr.* **2006**, *144*, 484206.
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**BROMOCRESOL PURPLE, SODIUM SALT**

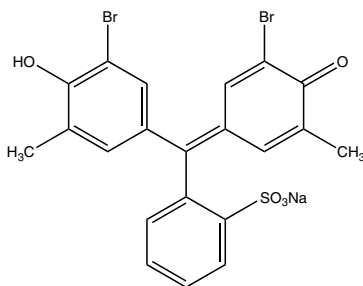
**Other Names** Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-methyl-, S,S-dioxide, monosodium salt; 3H-2,1-Benzoxathiole, phenol deriv.

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-methyl-, monosodium salt

**CAS Registry Number** 62625-30-3

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>21</sub>H<sub>15</sub>Br<sub>2</sub>O<sub>5</sub>SNa

**Molecular Weight** 562.22

**pH Range** 5.2–6.8

**Color Change at pH** Yellow (5.2) to purple (6.8)

**pKa** 6.3, 6.12

**Physical Form** Brownish-black crystalline powder

**Solubility** Soluble in water, ethanol

**UV-Visible (λ<sub>max</sub>)** 585 nm, 379 nm

**Melting Point** 255°C (decompose)

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Study properties of silicon dioxide films<sup>1</sup>

**Safety/Toxicity** No data available

**Reference**

1. Murashkevich, A. N.; Vashina, V. G.; Zharskii, I. M. Structural-sorption properties of films of SiO<sub>2</sub>. *Seryya Khim. Navuk* **2002**, 10–16; *Chem. Abstr.* **2002**, 137, 68531.

## BROMOPHENOL BLUE

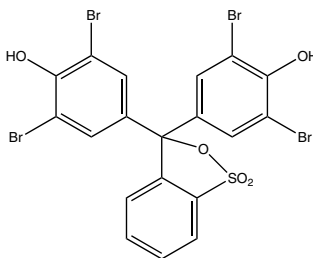
**Other Names** Bromophenol Blue; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-, S,S-dioxide; 3H-2,1-Benzoxathiole, phenol deriv.; 3',3'',5',5''-Tetrabromophenolsulfophthalein; Albutest; Bromphenol blue; NSC 7818; Tetrabromophenolsulfophthalein

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-

**CAS Registry Number** 115-39-9

**Merck Index Number** 1444

**Chemical Structure**



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>19</sub>H<sub>10</sub>Br<sub>4</sub>O<sub>5</sub>S

**Molecular Weight** 669.96

**pH Range** 3.0–4.6

**Color Change at pH** Yellow (3.0) to blue-purple (4.6)

**pKa** 4.0, 3.85, 3.6

**Physical Form** Yellowish-brownish powder

**Solubility** Sparingly soluble in water; soluble in ethanol, methanol, benzene

**UV-Visible (λ<sub>max</sub>)** 598 nm, 592 nm, 436 nm, 422 nm, 273 nm

**Melting Point** 279°C (decompose)

**Boiling Point (Calcd.)** 605.6 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Nanotechnology,<sup>6</sup> semiconductors,<sup>7</sup> sol-gel matrix,<sup>8</sup> fuel cells,<sup>9</sup> display device,<sup>10</sup> paints,<sup>11</sup> packaging system,<sup>12</sup> diapers,<sup>13</sup> contact lens,<sup>14</sup> determining nucleic acids,<sup>15</sup> mucin in saliva,<sup>16</sup> water alkalinity,<sup>17</sup> preserving genetic materials,<sup>18</sup> detecting bacteria,<sup>19</sup> vaginal infection test method<sup>20</sup>

**Safety/Toxicity** Toxicology,<sup>21</sup> mutagenicity,<sup>22</sup> toxicity<sup>23</sup>

## References

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- B**
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  12. Stecklein, G.; Duski, M.; Rozycki, A. G. Packaging system for a sterilized article. U.S. Pat. Appl. Publ. US 2006088450, 2006; *Chem. Abstr.* **2006**, *144*, 398463.
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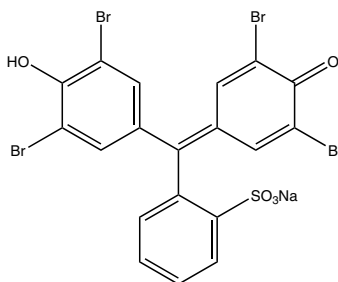
**BROMOPHENOL BLUE, SODIUM SALT**

**Other Names** Phenol, 4,4'-(3H-1,2-benzoxathiol-3-ylidene)bis[2,6-dibromo-,S,S-dioxide, mono-sodium salt; 3H-1,2-Benzoxathiole, phenol deriv.

**CA Index Name** Phenol, 4,4'-(2,2-dioxido-3H-1,2-benzoxathiol-3-ylidene)bis[2,6-dibromo-, mono-sodium salt

**CAS Registry Number** 62625-28-9

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>19</sub>H<sub>9</sub>Br<sub>4</sub>O<sub>5</sub>SNa

**Molecular Weight** 691.97

**pH Range** 3.0–4.6

**Color Change at pH** Yellow (3.0) to blue (4.6)

**pKa** 4.0, 3.85, 3.6

**Physical Form** Blue-black crystalline powder

**Solubility** Soluble in water, ethanol

**UV-Visible (λ<sub>max</sub>)** 589 nm, 383 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Recording materials<sup>4</sup>

**Safety/Toxicity** No data available

**References**

1. White, E. C.; Acree, S. F. On the quinone-phenolate theory of indicators: on the reactions of phenolsulfonephthalein, and its bromo and nitro derivatives, and their monobasic and dibasic salts. *J. Am. Chem. Soc.* **1919**, *41*, 1190–1212.
2. Orndorff, W. R.; Sherwood, F. W. Phenolsulfonephthalein and some of its derivatives. *J. Am. Chem. Soc.* **1923**, *45*, 486–500.
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## BROMOPHENOL RED

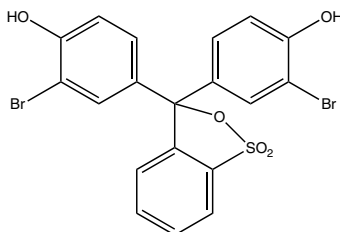
**Other Names** Bromophenol red; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)*bis*[2-bromo-, S,S-dioxide; *o*-Toluenesulfonic acid,  $\alpha,\alpha$ -*bis*(3-bromo-4-hydroxyphenyl)- $\alpha$ -hydroxy-,  $\gamma$ -sultone; 3H-2,1-Benzoxathiole, phenol deriv.; Bromophenol red

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*[2-bromo-

**CAS Registry Number** 2800-80-8

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>19</sub>H<sub>12</sub>Br<sub>2</sub>O<sub>5</sub>S

**Molecular Weight** 512.17

**pH Range** 5.2–6.8

**Color Change at pH** Yellow (5.2) to red (6.8)

**pKa** 6.51

**Physical Form** Reddish-brown powder

**Solubility** Sparingly soluble in water; soluble in ethanol

**UV-Visible ( $\lambda_{\text{max}}$ )** 574 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 586.8  $\pm$  50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Sensors,<sup>3,4</sup> sol-gel matrix,<sup>5</sup> recording materials,<sup>6</sup> thermochromic materials,<sup>7</sup> inks,<sup>8</sup> paints,<sup>9</sup> alloy coatings,<sup>10</sup> lubricants,<sup>11</sup> soaps,<sup>12</sup> cosmetics,<sup>13</sup> identifying fresh & stale rice,<sup>14</sup> determining acidity in wine,<sup>15</sup> food storage,<sup>16</sup> determination of bacterial growth,<sup>17</sup> anti-amyloid agents,<sup>18,19</sup> evaluating dental caries activity,<sup>20,21</sup> determination of *Streptococci* in human saliva,<sup>22</sup> diagnosis of enterohemorrhagic *Escherichia coli*,<sup>23</sup> treatment of acute leukemia<sup>24</sup>

**Safety/Toxicity** No data available

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- Sumina, E. G.; Shtykov, S. N.; Tyurina, N. V. Physicochemical aspects of micellar thin-layer chromatography. *Zh. Fiz. Khim.* **2002**, *76*, 1697–1702; *Chem. Abstr.* **2002**, *138*, 214653.
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## BROMOTHYMOL BLUE

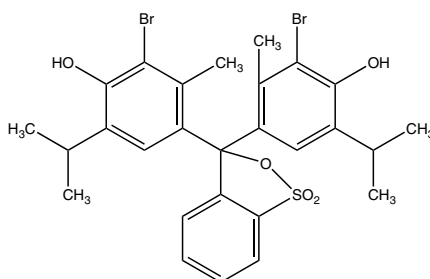
**Other Names** Bromothymol blue; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-3-methyl-6-(1-methylethyl)-, S,S-dioxide; Thymol, 6,6'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-, S,S-dioxide; 3H-2,1-Benzoxathiole, phenol deriv.; 3,3'-Dibromothymolsulfonphthalein; 3,3'-Dibromothymolsulfophthalein; Bromthymol blue; Dibromothymolsulfophthalein; NSC 7819

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-3-methyl-6-(1-methylethyl)-

**CAS Registry Number** 76-59-5

**Merck Index Number** 1445

**Chemical Structure**



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula**  $C_{27}H_{28}Br_2O_5S$

**Molecular Weight** 624.38

**pH Range** 6.0–7.6

**Color Change at pH** Yellow (6.0) to blue (7.6)

**pKa** 7.0, 7.1

**Physical Form** Light pink or cream colored powder

**Solubility** Sparingly soluble in water, benzene; soluble in ethanol, ether; insoluble in petroleum ether

**UV-Visible ( $\lambda_{max}$ )** 420 nm, 435 nm, 620 nm

**Melting Point** 201°C

**Boiling Point (Calcd.)**  $614.3 \pm 55.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Sol-gel matrix,<sup>6</sup> fuel cells,<sup>7</sup> optical sensors,<sup>8</sup> combustion gas detection system,<sup>9</sup> paints,<sup>10</sup> toys,<sup>11</sup> cleaning products,<sup>12</sup> detergents,<sup>13</sup> textiles,<sup>14</sup> food freshness sensor,<sup>15</sup> identifying fresh and stale rice,<sup>16</sup> wheat,<sup>17</sup> detecting microorganisms,<sup>18</sup> bacterial growth,<sup>19</sup> psychoactive drug,<sup>20</sup> dental materials<sup>21</sup>

**Safety/Toxicity** Toxicity<sup>22</sup>

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## BROMOTHYMOL BLUE, SODIUM SALT

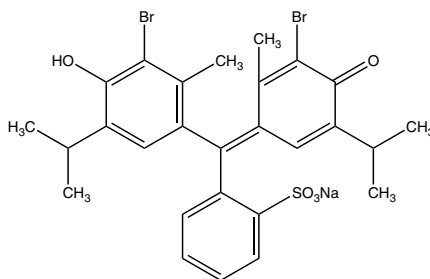
**Other Names** Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)*bis*[2-bromo-3-methyl-6-(1-methylethyl)-, S,S-dioxide, monosodium salt; 3H-2,1-Benzoxathiole, phenol deriv.; Bromthymol blue sodium

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*[2-bromo-3-methyl-6-(1-methylethyl)-, monosodium salt

**CAS Registry Number** 34722-90-2

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>27</sub>H<sub>27</sub>Br<sub>2</sub>O<sub>5</sub>SNa

**Molecular Weight** 646.38

**pH Range** 6.0–7.6

**Color Change at pH** Yellow (6.0) to blue (7.6)

**pKa** 7.0, 7.1

**Physical Form** Orange-brown powder

**Solubility** Soluble in water, ethanol

**UV-Visible (λ<sub>max</sub>)** 615 nm, 392 nm

**Melting Point** >250°C

**Synthesis** Synthetic method<sup>1,2</sup>

**Major Applications** Lithium battery,<sup>3</sup> textiles,<sup>2</sup> antagonists<sup>4</sup>

**Safety/Toxicity** No data available

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## BROMOXYLENOL BLUE

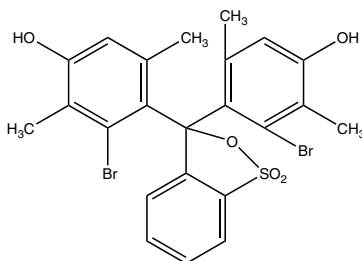
**Other Names** Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[3-bromo-2,5-dimethyl-, S,S-dioxide; 3H-2,1-Benzoxathiole, phenol deriv.; 3,3'-Dibromo-*p*-xylenolsulfophthalein; 4,4'-(3H-2,1-Benzoxathiol-3-ylidene)bis[3-bromo-2,5-dimethylphenol] S,S-dioxide; Bromoxyleneol blue; Bromxyleneol blue

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[3-bromo-2,5-dimethyl-

**CAS Registry Number** 40070-59-5

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>23</sub>H<sub>20</sub>Br<sub>2</sub>O<sub>5</sub>S

**Molecular Weight** 568.27

**pH Range** 6.0–7.6

**Color Change at pH** Yellow (6.0) to blue (7.6)

**pKa** 7.0

**Physical Form** Violet powder

**Solubility** Slightly soluble in water, ethanol; soluble in ethyl acetate, acetone

**UV-Visible (λ<sub>max</sub>)** 417 nm

**Melting Point** 218°C (decompose)

**Boiling Point (Calcd.)** 642.8 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Optical lenses,<sup>2</sup> sol-gel matrix,<sup>3</sup> inks,<sup>4</sup> paints,<sup>4</sup> toys,<sup>4</sup> lubricants,<sup>5</sup> cosmetics,<sup>6</sup> food storage,<sup>7</sup> microorganism detector,<sup>8</sup> determination of drugs,<sup>9</sup> diagnosis of multiple diseases<sup>10</sup>

**Safety/Toxicity** No data available

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# C

## CALCEIN

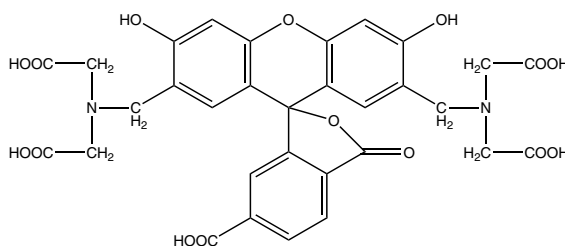
**Other Names** Fluorescein, 2',7'-bis[[bis(carboxymethyl)amino]methyl]-; Spiro[isobenzofuran-1(3H),9'-[9H]xanthene], glycine derivative; 2,7-Bis[*N,N*-bis(carboxymethyl)aminomethylene]-fluorescein; Acetic acid, [(3',6'-dihydroxy-2',7'-fluorandiyl)bis-(methylenenitrilo)]tetra-; Calcein; Fluorescein complexon; Fluorexon; NSC 298193; Oftasceine

**CA Index Name** Glycine, *N,N'*-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-2',7'-diyl)bis(methylene)]bis[*N*-(carboxymethyl)-

**CAS Registry Number** 1461-15-0

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>30</sub>H<sub>26</sub>N<sub>2</sub>O<sub>13</sub>

**Molecular Weight** 622.53

**pH Range** 6.0–7.2

**Color Change at pH** Weak green fluorescence (6.0) to strong green fluorescence (7.2)

**pKa** 6.67

**Physical Form** Orange powder

**Solubility** Soluble in water, ethanol

**UV-Visible (λ<sub>max</sub>)** 494 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 952.7 ± 65.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1-6</sup>

**Major Applications** Chemical-mechanical polishing,<sup>7,8</sup> stabilizing liposomes,<sup>9</sup> cell motility assay,<sup>10</sup> detecting nucleic acids,<sup>11</sup> virus,<sup>12</sup> screening safety of gastric mucosa,<sup>13</sup> MDR inhibitors,<sup>14</sup> drug delivery,<sup>15</sup> imaging atherosclerotic plaque<sup>16</sup>

**Safety/Toxicity** Cytotoxicity,<sup>17</sup> exitotoxicity<sup>18</sup>

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**CALMAGITE**

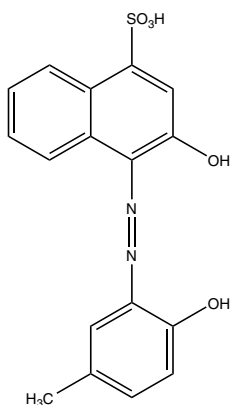
**Other Names** 1-Naphthalenesulfonic acid, 3-hydroxy-4-[(6-hydroxy-*m*-tolyl)azo]-; 2-Naphthol-4-sulfonic acid, 1-(6-hydroxy-*m*-tolylazo); 1-(1-Hydroxy-4-methyl-2-phenylazo)-2-naphthol-4-sulfonic acid; 1-(1-Hydroxy-4-methyl-4-phenylazo)-2-naphthol-4-sulfonic acid; 1-[(2-Hydroxy-5-methylphenyl)azo]-2-naphthol-4-sulfonic acid; 3-Hydroxy-4-[(6-hydroxy-*m*-tolyl)azo]-1-naphthalenesulfonic acid; Calmagite; NSC 299391

**CA Index Name** 1-Naphthalenesulfonic acid, 3-hydroxy-4-[(2-hydroxy-5-methylphenyl)azo]-

**CAS Registry Number** 3147-14-6

**Merck Index Number** 1718

**Chemical Structure**



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>17</sub>H<sub>14</sub>N<sub>2</sub>O<sub>5</sub>S

**Molecular Weight** 358.37

**pH Range** 7.1–9.1

**Color Change at pH** Red (7.1) to blue (9.1)

**pKa** 8.1

**Physical Form** Red-blackish crystals

**Solubility** Soluble in water, ethanol

**UV-Visible (λ<sub>max</sub>)** 610 nm

**Melting Point** 300°C

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Nanoparticles,<sup>3</sup> cleaning microelectronic substrates,<sup>4</sup> sensors,<sup>5</sup> photographic materials,<sup>6</sup> recording materials,<sup>7</sup> water hardness measurement,<sup>8</sup> indicator for calcium and magnesium,<sup>9</sup> determination of vanadium,<sup>10</sup> medical component,<sup>11</sup> measuring magnesium in biological fluids,<sup>12</sup> diagnosis of diseases caused by elemental imbalance,<sup>13</sup> treatment of thrombocytopenia,<sup>14</sup> urine analysis test strip<sup>15</sup>

**Safety/Toxicity** No data available

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**CARBAZOL YELLOW**

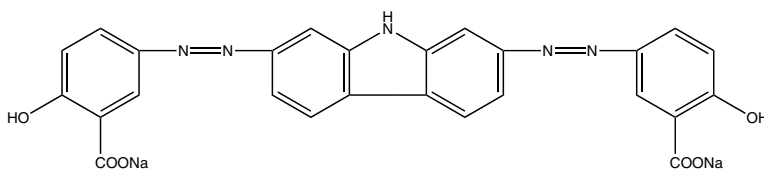
**Other Names** Salicylic acid, 5,5'-[carbazole-2,7-diylbis(azo)]di-, disodium salt; C.I. 25700; Carbazol Yellow

**CA Index Name** Benzoic acid, 3,3'-[9H-carbazole-2,7-diylbis(azo)]bis[6-hydroxy-, disodium salt

**CAS Registry Number** 6411-46-7

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>26</sub>H<sub>15</sub>N<sub>5</sub>O<sub>6</sub>Na<sub>2</sub>

**Molecular Weight** 539.40

**pH Range** 12.0–14.0

**Color Change at pH** Yellow (12.0) to red (14.0)

**pKa** 13.7

**Physical Form** Yellow crystals

**Solubility** Soluble in water, ethanol

**Melting Point** >250°C

**Synthesis** No data available

**Major Applications** No data available

**Safety/Toxicity** No data available

**References** No reference available



## 5-CARBOXYFLUORESCEIN

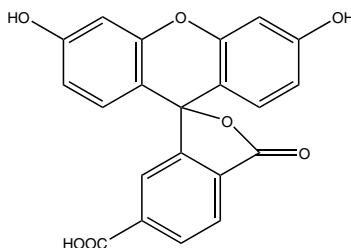
**Other Names** 5-Carboxyfluorescein; FAM; FAM (dye); FAM 494/520

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid,3',6'-dihydroxy-3-oxo-

**CAS Registry Number** 76823-03-5

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula**  $C_{21}H_{12}O_7$

**Molecular Weight** 376.32

**pH Range** 6.0–7.2

**Color Change at pH** Weak green fluorescence (6.0) to strong green fluorescence (7.2)

**pKa** 3.3, 4.6, 6.4, 7.0

**Physical Form** Solid

**Solubility** Soluble in water, *N,N*-dimethylformamide

**UV-Visible ( $\lambda_{max}$ )** 492 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)**  $725.2 \pm 60.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1-3</sup>

**Major Applications** Fluorescent probe,<sup>4</sup> diagnosis of cancer,<sup>5</sup> leukemia,<sup>6</sup> colorectal cancer,<sup>7</sup> polynucleotide,<sup>8</sup> bacteria,<sup>9</sup> pathogens,<sup>10</sup> nucleic acid,<sup>11</sup> hepatitis A virus,<sup>12</sup> dengue virus,<sup>13</sup> herpes simplex virus,<sup>14</sup> gene,<sup>15</sup> HIV type,<sup>16</sup> cardiovascular risk factor<sup>17</sup>

**Safety/Toxicity** Genotoxicity<sup>18</sup>

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## 6-CARBOXYFLUORESCEIN

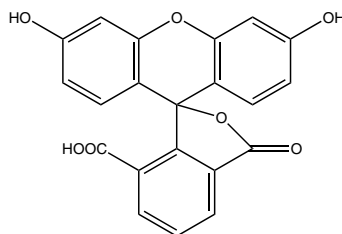
**Other Names** Spiro[phthalan-1,9'-xanthene]-6-carboxylic acid,3',6'-dihydroxy-3-oxo-; Terephthalic acid, (3,6,9-trihydroxyxanthen-9-yl)-,  $\gamma$ -lactone; 6-Carboxyfluorescein; 6-FAM; 6-carboxyfluorescein; Fluorescein, 6-carboxy-

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid,3',6'-dihydroxy-3-oxo-

**CAS Registry Number** 3301-79-9

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula**  $C_{21}H_{12}O_7$

**Molecular Weight** 376.32

**pH Range** 6.0–7.2

**Color Change at pH** Weak green fluorescence (6.0) to strong green fluorescence (7.2)

**pKa** 3.3, 4.6, 6.4, 7.0

**Physical Form** Solid

**Solubility** Soluble in water, *N,N*-dimethylformamide

**UV-Visible ( $\lambda_{max}$ )** 492 nm

**Melting Point** >360°C

**Boiling Point (Calcd.)**  $736.4 \pm 60.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Diagnosis of hematologic cancer,<sup>3</sup> nongastric diseases,<sup>4</sup> detection of genetically modified wheat,<sup>5</sup> chromosomes,<sup>6</sup> gene expression,<sup>7</sup> nucleic acid,<sup>8</sup> hepatitis A virus,<sup>9</sup> avian influenza virus subtype H5 and H5N1,<sup>10</sup> SARS virus,<sup>11</sup> herpes simplex virus<sup>12</sup>

**Safety/Toxicity** Cytotoxicity,<sup>13</sup> genotoxicity,<sup>14</sup> immunotoxicity<sup>15</sup>

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## 5-CARBOXYFLUORESC EIN DIACETATE

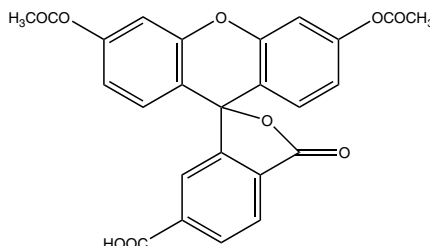
**Other Names** 5-Carboxyfluorescein diacetate

**CA Index Name** Spiro[isobenzofuran-1(3H),9′-[9H]xanthene]-5-carboxylic acid,3′,6′-bis(acetyloxy)-3-oxo-

**CAS Registry Number** 79955-27-4

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>25</sub>H<sub>16</sub>O<sub>9</sub>

**Molecular Weight** 460.39

**pH Range** 6.0–7.2

**Color Change at pH** Weak green fluorescence (6.0) to strong green fluorescence (7.2)

**pKa** 6.4

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in dimethyl sulfoxide

**UV-Visible (λ<sub>max</sub>)** <300 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 693.1 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–9</sup>

**Major Applications** Sensors,<sup>10</sup> method for measuring bacteria,<sup>11</sup> detecting intracellular pH in yeast,<sup>12</sup> determination of extracellular and intracellular pH of microorganisms,<sup>13</sup> detecting living cells,<sup>14,15</sup> identification of cancerous cells,<sup>16</sup> method for assessing microorganism viability,<sup>17</sup> determining proliferative activities in tumor tissues,<sup>18</sup> measuring the growth of keratinocytes,<sup>19</sup> antifungal agent,<sup>20,21</sup> neurodegenerative disorders,<sup>22</sup> antineoplastic drugs<sup>23</sup>

**Safety/Toxicity** No data available

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## 6-CARBOXYFLUORESC EIN DIACETATE

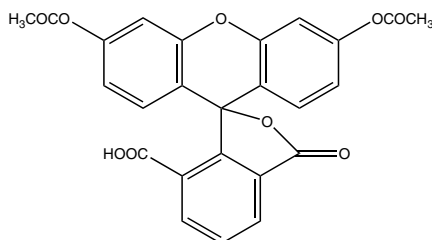
**Other Names** Spiro[phthalan-1,9'-xanthene]-6-carboxylic acid, 3',6'-dihydroxy-3-oxo-, diacetate; Terephthalic acid, (3,6,9-trihydroxyxanthen-9-yl)-,  $\gamma$ -lactone, diacetate; 6-Carboxyfluorescein diacetate

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid,3',6'-bis (acetyloxy)-3-oxo-

**CAS Registry Number** 3348-03-6

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula**  $C_{25}H_{16}O_9$

**Molecular Weight** 460.39

**pH Range** 6.0–7.2

**Color Change at pH** Weak green fluorescence (6.0) to strong green fluorescence (7.2)

**pKa** 6.4

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in dimethyl sulfoxide

**UV-Visible ( $\lambda_{max}$ )** <300 nm

**Melting Point** 152–153°C

**Boiling Point (Calcd.)** 701.6  $\pm$  60.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Fluorescent probes,<sup>4</sup> detecting cells,<sup>5</sup> microorganisms,<sup>5</sup> yeasts,<sup>6</sup> antifungal agent,<sup>7</sup> antibacterials agent<sup>8</sup>

**Safety/Toxicity** Ploem mobility of xenobiotics,<sup>9</sup> retinal toxicity<sup>10</sup>

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## 5(6)-CARBOXYFLUORESC EIN DIACETATE SUCCINIMIDYL ESTER

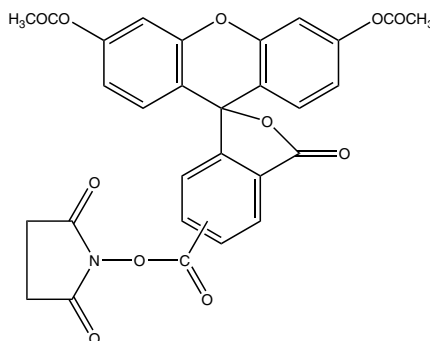
**Other Names** Spiro[isobenzofuran-1(3H),9'-[9H]xanthene], 2,5-pyrrolidinedione derivative; 5-(6)-Carboxyfluorescein diacetate succinimidyl ester

**CA Index Name** 2,5-Pyrrolidinedione, 1-[[[3',6'-bis(acetyloxy)-3-oxospiro-[isobenzofuran-1(3H),9'-[9H]xanthen]-5(or 6)-yl]carbonyl]oxy]-

**CAS Registry Number** 150347-59-4

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>29</sub>H<sub>19</sub>NO<sub>11</sub>

**Molecular Weight** 557.47

**pH Range** 6.0–7.2

**Color Change at pH** Weak green fluorescence (6.0) to strong green fluorescence (7.2)

**pKa** 6.45

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in *N,N*-dimethylformamide, dimethyl sulfoxide

**UV-Visible (λ<sub>max</sub>)** <300

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Diagnosis of cancer,<sup>4</sup> restricting HIV replication,<sup>5</sup> antiinflammatory agent,<sup>6</sup> detecting bacteria,<sup>7</sup> cell proliferation assays<sup>8</sup>

**Safety/Toxicity** No data available

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8. Hu, H.; Puchalski, A. Cell proliferation assays and methods. U.S. Pat. Appl. Publ. US 2003228635, 2003; *Chem. Abstr.* **2003**, 140, 2543.

## 5-CARBOXYNAPHTHOFLUORESCIN

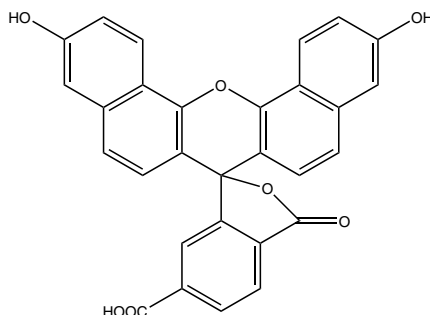
**Other Names** 5-Carboxynaphthofluorescein

**CA Index Name** Spiro[7H-dibenzo[c,h]xanthene-7,1'(3'H)-isobenzofuran]-5'-carboxylic acid, 3,6a-dihydro-11-hydroxy-3,3'-dioxo-

**CAS Registry Number** 145103-60-2

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>29</sub>H<sub>16</sub>O<sub>7</sub>

**Molecular Weight** 476.43

**pH Range** 6.0–9.0

**Color Change at pH** Weak red fluorescence (6.0) to strong red fluorescence (9.0)

**pKa** 7.6

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in *N,N*-dimethylformamide

**UV-Visible (λ<sub>max</sub>)** 512 nm, 598 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 845.9 ± 65.0°C Pressure: 760 Torr

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Sensors,<sup>2–5</sup> organic electroluminescence (OEL)-based biochips,<sup>6,7</sup> method for detecting fluorescent molecule,<sup>8</sup> fluorescence studies of protein crystal nucleation<sup>9</sup>

**Safety/Toxicity** No data available

## References

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## 6-CARBOXYNAPHTHOFLOURESC EIN

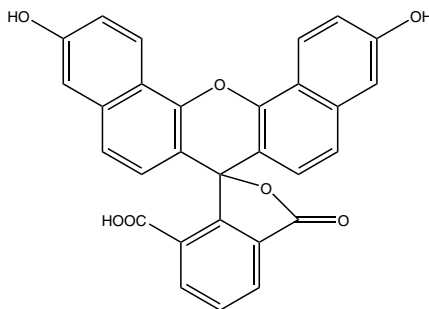
**Other Names** 6-Carboxynaphthofluorescein

**CA Index Name** Spiro[7H-dibenzo[c,h]xanthene-7,1'(3'H)-isobenzofuran]-4'-carboxylic acid, 3,11-dihydro-3'-oxo-

**CAS Registry Number** 145103-61-3

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>29</sub>H<sub>16</sub>O<sub>7</sub>

**Molecular Weight** 476.43

**pH Range** 6.0–9.0

**Color Change at pH** Weak red fluorescence (6.0) to strong red fluorescence (9.0)

**pKa** 7.6

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in *N,N*-dimethylformamide

**UV-Visible (λ<sub>max</sub>)** 512 nm, 598 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 851.4 ± 65.0°C Pressure: 760 Torr

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Sensors,<sup>2–5</sup> organic electroluminescence (OEL)-based biochips,<sup>6,7</sup> fluorescence studies of protein crystal nucleation<sup>8</sup>

**Safety/Toxicity** No data available

## References

1. Wolfbeis, O. S.; Rodriguez, N. V.; Werner, T. LED-compatible fluorosensor for measurement of near-neutral pH values. *Mikrochim. Acta* **1992**, 108, 133–141.
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5. Bentsen, J. G.; Wood, K. B. Sensor with improved drift stability. US Patent 5403746, 1995; *Chem. Abstr.* **1995**, 123, 73757.
6. Jang, S.; Suen, S.; Chen, S.; Lin, C.; Yang, J. Organic electroluminescence (OEL)-based biochips. Taiwan Patent TW 504945, 2002; *Chem. Abstr.* **2004**, 140, 371431.
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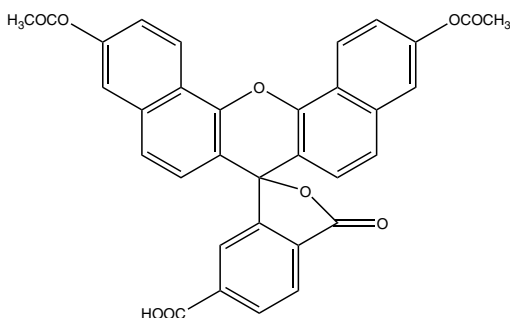
**5-CARBOXYNAPHTHOFLUORESCEIN DIACETATE**

**Other Names** 5-Carboxynaphthofluorescein diacetate

**CA Index Name** Spiro[7H-dibenzo[c,h]xanthene-7,1'(3'H)-isobenzofuran]-5'-carboxylic acid, 3,11-bis(acetyloxy)-3'-oxo-

**CAS Registry Number** 164256-07-9

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>33</sub>H<sub>20</sub>O<sub>9</sub>

**Molecular Weight** 560.51

**pH Range** 6.0–9.0

**Color Change at pH** Weak red fluorescence (6.0) to strong red fluorescence (9.0)

**pKa** 7.6

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in dimethyl sulfoxide

**UV-Visible (λ<sub>max</sub>)** <300 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 828.4 ± 65.0°C Pressure: 760 Torr

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Sensors<sup>1</sup>

**Safety/Toxicity** No data available

**Reference**

1. Bentsen, J. G.; Wood, K. B. Sensor with improved drift stability. US Patent 5403746, 1995; *Chem. Abstr.* **1995**, 123, 73757.

## CARBOXY SNAFL 1

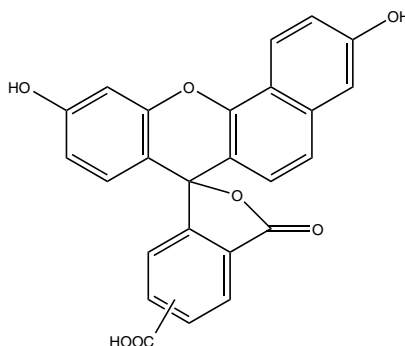
**Other Names** Carboxy SNAFL 1

**CA Index Name** Spiro[7H-benzo[c]xanthene-7,1'(3'H)-isobenzofuran]-ar'-carboxylic acid, 3, 10-dihydroxy-3'-oxo-

**CAS Registry Number** 134344-20-0

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>25</sub>H<sub>14</sub>O<sub>7</sub>

**Molecular Weight** 426.38

**pH Range** 6.0–9.0

**Color Change at pH** Weak green fluorescence (6.0) to strong green fluorescence (9.0)

**pKa** 7.8

**Physical Form** Solid

**Solubility** Soluble in water

**UV-Visible (λ<sub>max</sub>)** 508 nm

**Melting Point** >250°C

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** pH Sensors,<sup>1</sup> optical chemical sensors,<sup>2</sup> biochemical sensors,<sup>3</sup> biosensors,<sup>4</sup> fluorescent pH detector system,<sup>5</sup> measuring fluorescence lifetime in cells,<sup>6</sup> determining concentration of a laminar sample stream,<sup>7</sup> fluorescent reporter beads for fluid analysis,<sup>8</sup> measuring chemical analytes,<sup>9</sup> intracellular pH in human sperms,<sup>10</sup> multidrug resistance,<sup>11</sup> recording intramitochondrial pH,<sup>12</sup> fluorescent probes<sup>13</sup>

**Safety/Toxicity** Toxicity in root phloem<sup>14</sup>

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## CARBOXY SNAFL 2

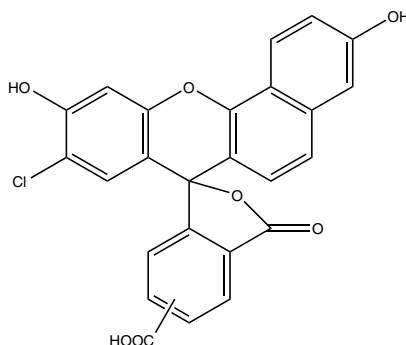
**Other Names** 10H-Benzo[c]xanthene, benzenedicarboxylic acid derivative; Carboxy-SNAFL 2

**CA Index Name** Benzenedicarboxylic acid, (9-chloro-3-hydroxy-10-oxo-10H-benzo[c]xanthen-7-yl)-

**CAS Registry Number** 146472-79-9

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent

**Molecular Formula**  $C_{25}H_{13}ClO_7$

**Molecular Weight** 460.83

**pH Range** 6.0–9.0

**Color Change at pH** Weak green fluorescence (6.0) to strong green fluorescence (9.0)

**pKa** 7.7

**Physical Form** Solid

**Solubility** Soluble in water

**UV-Visible ( $\lambda_{max}$ )** 514 nm

**Melting Point**  $>250^\circ\text{C}$

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Sensors,<sup>2</sup> measuring chemical analytes,<sup>3</sup> fluorescence lifetime in cells,<sup>4</sup> fluorescent pH detector system<sup>5</sup>

**Safety/Toxicity** No data available

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4. Andersson, R. M.; Carlsson, K.; Liljeborg, A.; Brismar, H. Fluorescence lifetime imaging of pH in cells: investigation of factors influencing the pH calibration lifetime. *Proc. SPIE-Int. Soc. Opt. Eng.* **2000**, *3921*, 242–248.
5. Reed, M. W.; Geelhood, S. J.; Harris, P. C.; Pfalzgraf, R. D. Fluorescent pH detector system and related methods. PCT Int. Appl. WO 2006023725, 2006; *Chem. Abstr.* **2006**, *144*, 270133.

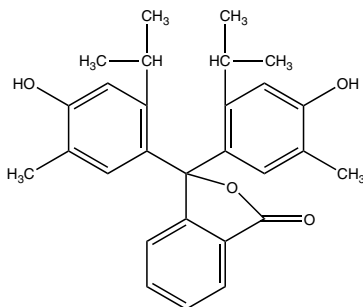
**CARVACROLPHTHALEIN**

**Other Names** Phenolphthalein, 2',2''-diisopropyl-5',5''-dimethyl-;

**CA Index Name** 1(3H)-Isobenzofuranone, 3,3-bis[4-hydroxy-5-methyl-2-(1-methylethyl)phenyl]-

**CAS Registry Number** 6869-00-7

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Phthalein

**Molecular Formula** C<sub>28</sub>H<sub>30</sub>O<sub>4</sub>

**Molecular Weight** 430.54

**pH Range** 9.5–10.0

**Color Change at pH** Colorless (9.5) to blue (10.0)

**pKa** 9.69

**Physical Form** Colorless crystals

**Solubility** Almost insoluble in water; soluble in ethanol

**Melting Point** 294°C

**Boiling Point (Calcd.)** 598.9 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Laxatives<sup>3,4</sup>

**Safety/Toxicity** No data available

**References**

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## CHLOROPHENOL RED

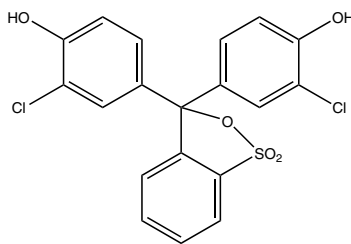
**Other Names** Chlorophenol red; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-chloro-, S,S-dioxide; *o*-Toluenesulfonic acid,  $\alpha,\alpha$ -bis(3-chloro-4-hydroxyphenyl)- $\alpha$ -hydroxy-,  $\gamma$ -sultone; 3H-2,1-Benzoxathiole, phenol derivative; Chlorphenol red; Chlorphenolsulfonphthalein; Dichlorophenolsulfonephthalein; NSC 7828

**CA Index Name:** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-chloro-

**CAS Registry Number** 4430-20-0

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula**  $C_{19}H_{12}Cl_2O_5S$

**Molecular Weight** 423.27

**pH Range** 4.8–6.4

**Color Change at pH** Yellow (4.8) to red (6.4)

**pKa** 6.0

**Physical Form** Brownish-red or brownish-green powder

**Solubility** Sparingly soluble in water; soluble in ethanol

**UV-Visible ( $\lambda_{max}$ )** 572 nm

**Melting Point** 261–262°C

**Boiling Point (Calcd.)**  $583.0 \pm 50.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Waveguide,<sup>6</sup> sol-gel matrix,<sup>7</sup> display device,<sup>8</sup> tin electroplating process,<sup>9</sup> inks,<sup>10</sup> lubricants,<sup>11</sup> detergents,<sup>12</sup> preservation of cut flowers,<sup>13</sup> cosmetics,<sup>14</sup> identifying fresh and stale rice,<sup>15</sup> determining acidity in wine,<sup>16</sup> food storage,<sup>17</sup> detecting lactic acid bacteria,<sup>18</sup> enzyme assays,<sup>19</sup> diagnosis of bacterial and fungal infection,<sup>20</sup> oral hygiene products<sup>21</sup>

**Safety/Toxicity** Oestrogenic activity<sup>22</sup>

## References

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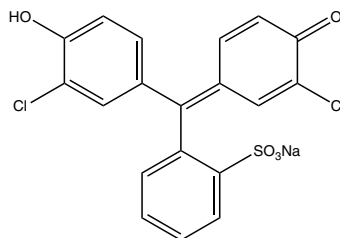
**CHLOROPHENOL RED, SODIUM SALT**

**Other Names** Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)*bis*[2-chloro-, *S,S*-dioxide, monosodium salt; Chlorophenol red, sodium salt

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*[2-chloro-, monosodium salt

**CAS Registry Number** 123333-64-2

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>19</sub>H<sub>11</sub>Cl<sub>2</sub>O<sub>5</sub>SNa

**Molecular Weight** 445.26

**pH Range** 4.8–6.4

**Color Change at pH** Yellow (4.8) to red (6.4)

**pKa** 6.0

**Physical Form** Brown crystals

**Solubility** Soluble in water, ethanol

**UV-Visible (λ<sub>max</sub>)** 575 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Aerogel materials,<sup>1</sup> photoreceptors<sup>2</sup>

**Safety/Toxicity** No data available

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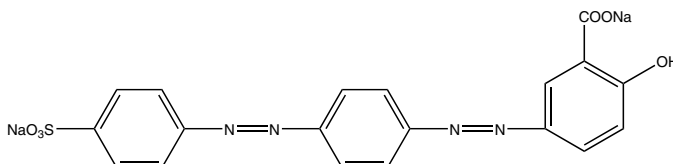
## CHROME ORANGE GR

**Other Names** C.I. Mordant Orange 6; C.I. Mordant Orange 6, disodium salt; Salicylic acid, 5-[*p*-(*p*-sulfophenylazo)phenylazo]-, disodium salt; Acid Chrome Orange GR; Acid Leather Orange CG; Alizarine Chrome Orange GR; Anthracene Orange G; Anthranol Chrome Orange GR; Atlantichrome Orange G; Azochromol Orange AS; Belachrome Fast Orange GR; Brilliant Orange; Brilliant Orange (indicator); C.I. 26520; C.I. Mordant Orange 44; Calcochrome Orange GR; Chromaven Milling Orange G; Chrome Fast Orange G; Chrome Fast Orange GR; Chrome orange; Chrome orange (Russian); Chromocard Orange 3R; Cromal Orange G; Cromal Orange P; Diacromo Orange GR; Diamond Chrome Orange GR; Durochrome Orange G; Eriochrome Orange G; Eriochrome Orange R; Hispacrom Fast Orange GR; Java Chrome Orange EN; Java Unichrome Orange E; Magracrom Orange GR; Mitsui Chrome Orange GR; Monochrome Brilliant Orange GR; Monochrome Orange GR; Naphthalene Leather Yellow R; Neutral Fast Orange G; Omega Chrome Orange G; Solochrome Leather Orange GR; Solochrome Orange GR; Solochrome Orange RS; Sunchromine Orange GR; Synchromate Orange G; Telon Chrome Orange G; Tetrochrome Orange GR; Wool Fast Orange GA-CF; Yodochrome Fast Orange GR

**CA Index Name** Benzoic acid, 2-hydroxy-5-[[4-[(4-sulfophenyl)azo]phenyl]azo]-, disodium salt

**CAS Registry Number** 3564-27-0

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{19}H_{12}N_4O_6SNa_2$

**Molecular Weight** 470.38

**pH Range** 10.5–12.0

**Color Change at pH** Yellow (10.5) to red (12.0)

**pKa** 11.49, 11.71

**Physical Form** Orange powder

**Solubility** Soluble in water; very slightly soluble in ethanol, acetone

**UV-Visible ( $\lambda_{max}$ )** 381 nm

**Melting Point**  $>300^\circ\text{C}$

**Synthesis** Synthetic method<sup>1,2</sup>

**Major Applications** Wool dyeing,<sup>3–5</sup> soy sauce,<sup>6</sup> antiAIDS agents<sup>7</sup>

**Safety/Toxicity** No data available

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## CHRYSOIDIN

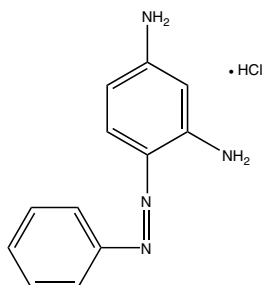
**Other Names** C.I. Basic Orange 2; C.I. Basic Orange 2, monohydrochloride; 2,4-Diaminoazobenzene hydrochloride; Astra Chrysoidine R; Atlantic Chrysoidine Y; Basic Orange 2; Basonyl Orange 200; Brasilazina Orange Y; C.I. 11270; Calcozine Orange YS; Chrysoidin; Chrysoidin FB; Chrysoidine; Chrysoidine A; Chrysoidine B; Chrysoidine C; Chrysoidine G; Chrysoidine GN; Chrysoidine GS; Chrysoidine HR; Chrysoidine II; Chrysoidine J; Chrysoidine M; Chrysoidine PRL; Chrysoidine PRR; Chrysoidine SL; Chrysoidine SS; Chrysoidine Y; Chrysoidine Y Crystals; Chrysoidine Y Special; Chrysoidine YL; Chrysoidine YN; Chrysoidine hydrochloride; Chrysoidine orange; Diazocard Chrysoidine G; Leather Orange HR; Nippon Kagaku Chrysoidine; Pure Chrysoidine YBH; Sugai Chrysoidine; Tertrophene Brown CG; Verona Chrysoidine GN

**CA Index Name** 1,3-Benzenediamine, 4-(phenylazo)-, monohydrochloride

**CAS Registry Number** 532-82-1

**Merck Index Number** 2257

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>12</sub>H<sub>12</sub>N<sub>4</sub>·HCl

**Molecular Weight** 248.72

**pH Range** 4.0–7.0

**Color Change at pH** Orange (4.0) to yellow (7.0)

**Physical Form** Reddish-brown crystals

**Solubility** Soluble in water, ethanol, acetone, methyl cellosolve, xylene; practically insoluble in benzene

**UV-Visible (λ<sub>max</sub>)** 449 nm

**Melting Point** 118–118.5°C

**Boiling Point** 2262°C

**Synthesis** Synthetic methods<sup>1–4</sup>

**Major Applications** Recording materials,<sup>5</sup> waveguides,<sup>6</sup> thin solid films,<sup>7</sup> photographic materials,<sup>8</sup> printing plates,<sup>9</sup> inks,<sup>10–12</sup> toners,<sup>13</sup> detergents,<sup>14</sup> corrosion inhibitors,<sup>15</sup> rubber,<sup>16</sup> textiles,<sup>17–19</sup> hair dyes<sup>20</sup>

**Safety/Toxicity** Toxicological evaluation,<sup>21</sup> mutagenicity,<sup>22</sup> carcinogenicity<sup>23</sup>

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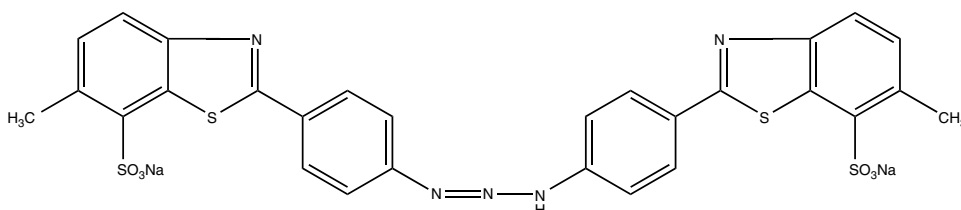
## CLAYTON YELLOW

**Other Names** C.I. Direct Yellow 9; C.I. Direct Yellow 9, disodium salt; Clayton Yellow; Atlantic Brilliant Yellow MN; Benzo Yellow TZ; C.I. 19540; Chlorazol Yellow 2G; Chlorazol Yellow DP; Diaphtamine Brilliant Yellow 6GS; Diazamine Golden Yellow T; Diazol Yellow J; Direct Yellow MTZ; Direct Yellow TZ; Ferro 42-145A; Hispamin Pure Yellow T2G; Mimosa Z; Peeramine Bright Yellow MN; Pontamine Pure Yellow; Pontamine Pure Yellow MN; Thiazol Yellow; Thiazol Yellow G; Thiazol Yellow GGM; Thiazol Yellow R; Thiazol Yellow Z; Thiazole Y; Thiazole Yellow G; Thiazole Yellow GGM; Thiazole yellow; Titan Yellow; Titan Yellow Dye; Titan Yellow G

**CA Index Name** 7-Benzothiazolesulfonic acid, 2,2'-(1-triazene-1,3-diyl-di-4,1-phenylene)bis[6-methyl-, disodium salt

**CAS Registry Number** 1829-00-1

**Merck Index Number** 9310

**Chemical Structure**

**Chemical/Dye Class** Azo, thiazole

**Molecular Formula**  $C_{28}H_{19}N_5O_6S_4Na_2$

**Molecular Weight** 695.73

**pH Range** 11.0–13.0

**Color Change at pH** Yellow (11.0) to red (13.0)

**Physical Form** Yellowish-brown powder

**Solubility** Soluble in water, ethanol

**UV-Visible ( $\lambda_{max}$ )** 402 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1-4</sup>

**Major Applications** Display device,<sup>5</sup> optical sensors,<sup>6,7</sup> thin-film device,<sup>8</sup> incandescent electric lamps,<sup>9</sup> photoreceptors,<sup>10</sup> lithographic process,<sup>11</sup> inks,<sup>12</sup> pencil leads,<sup>13</sup> paints,<sup>14</sup> adhesives,<sup>15</sup> plastic materials,<sup>16</sup> molding materials,<sup>17</sup> steel plates,<sup>18</sup> detection of albumin,<sup>19</sup> treatment of amyloidosis disorders,<sup>20</sup> treatment of apolipoprotein E-related diseases<sup>21</sup>

**Safety/Toxicity** Eye irritation test<sup>22</sup>

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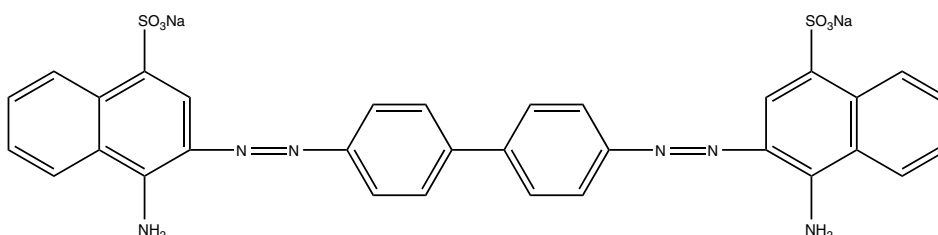
## CONGO RED

**Other Names** C.I. Direct Red 28, disodium salt; Atlantic Congo Red; Atul Congo Red; Azocard Red Congo; Benzo Congo Red; Brasilamina Congo 4B; C.I. 22120; C.I. Direct Red 28; Congo Red 4B; Congo Red 4BX; Congo Red CR; Congo Red H; Congo Red K; Congo Red L; Congo Red M; Congo Red N; Congo Red R; Congo Red RS; Congo Red W; Congo Red WS; Congo Red sodium salt; Congo red; Cotton Red 4BC; Cotton Red 5B; Cotton Red L; Diacotton Congo Red; Direct Congo Red; Direct Red 28; Direct Red C; Direct Red DC-CF; Direct Red K; Erie Congo 4B; Haemomedical; Haemonorm; Hemorrhagyl; Hispamin Congo 4B; Kayaku Congo Red; Mitsui Congo Red; Peeramine Congo Red; Red K; Solucongo; Sugai Congo Red; Tertrodirect Red C; Trisulfon Congo Red; Vondacel Red CL

**CA Index Name** 1-Naphthalenesulfonic acid, 3,3'-[[1,1'-biphenyl]-4,4'-diylbis-(azo)]bis[4-amino-, disodium salt

**CAS Registry Number** 573-58-0

**Merck Index Number** 2498

**Chemical Structure**

**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{32}H_{22}N_6O_6S_2Na_2$

**Molecular Weight** 696.67

**pH Range** 3.0–5.0

**Color Change at pH** Blue (3.0) to red (5.0)

**pKa** 4.1

**Physical Form** Brownish-red powder

**Solubility** Soluble in water, ethanol; very slightly soluble in acetone; practically insoluble in ether, xylene

**UV-Visible ( $\lambda_{max}$ )** 497 nm, 488 nm, 595 nm

**Melting Point**  $>360^\circ\text{C}$

**Synthesis** Synthetic methods<sup>1–9</sup>

**Major Applications** Waveguides,<sup>10</sup> optical sensors,<sup>11</sup> display devices,<sup>12</sup> inks,<sup>13</sup> fertilizer,<sup>14</sup> pesticides,<sup>15</sup> detecting carbohydrates,<sup>16</sup> treatment of pathogen infections,<sup>17</sup> age-related macular degeneration,<sup>18</sup> amyloid accumulation in the brain<sup>19</sup>

**Safety/Toxicity** Acute toxicity,<sup>20</sup> carcinogenicity,<sup>21</sup> cutaneous toxicity,<sup>22</sup> cytotoxicity,<sup>23</sup> genotoxicity,<sup>24</sup> mutagenicity,<sup>25</sup> neurotoxicity<sup>26</sup>

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## COUMARIN

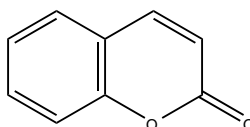
**Other Names** Coumarin; 1,2-Benzopyrone; 2-Propenoic acid, 3-(2-hydroxyphenyl)-,  $\delta$ -lactone; 5,6-Benzo-2-pyrone; Benzo- $\alpha$ -pyrone; Coumarinic anhydride; NSC 8774; Rattex; Tonka bean camphor; cis-*o*-Coumarinic acid lactone; *o*-Hydroxycinnamic acid lactone

**CA Index Name** 2H-1-Benzopyran-2-one

**CAS Registry Number** 91-64-5

**Merck Index Number** 2562

**Chemical Structure**



C

**Chemical/Dye Class** Fluorescent, Coumarin

**Molecular Formula** C<sub>9</sub>H<sub>6</sub>O<sub>2</sub>

**Molecular Weight** 146.14

**pH Range** 9.5–10.5

**Color Change at pH** Nonfluorescence (9.5) to light green fluorescence (10.5)

**Physical Form** White powder

**Solubility** Very slightly soluble in water; freely soluble in ethanol, ether, chloroform

**UV-Visible ( $\lambda_{\text{max}}$ )** 275 nm

**Melting Point** 68–70°C

**Boiling Point** 297–299°C

**Synthesis** Synthetic methods<sup>1–14</sup>

**Major Applications** Color filter,<sup>15</sup> organic electroluminescent devices,<sup>15,16</sup> liquid crystal displays,<sup>17</sup> field emission displays,<sup>18</sup> inks,<sup>19</sup> nickel plating,<sup>20</sup> detergents,<sup>21</sup> deodorant for shoes,<sup>22</sup> petroleum products,<sup>23</sup> cigarettes,<sup>24</sup> personal care products,<sup>25</sup> cosmetics,<sup>26</sup> sunscreen cream,<sup>27</sup> perfumes,<sup>28</sup> enzyme substrates,<sup>29</sup> nucleic acid sequencing,<sup>30</sup> antiinflammatory agent,<sup>31</sup> treatment of cancer,<sup>32</sup> neurotransmission disorders,<sup>33</sup> bleeding disorders,<sup>34</sup> cerebrovascular disease,<sup>35</sup> thrombosis,<sup>36</sup> hemorrhoids,<sup>37</sup> rheumatic disease,<sup>38</sup> arthritic disease,<sup>38</sup> epilepsy,<sup>39</sup> vaginitis,<sup>40</sup> painkiller,<sup>41</sup> teeth whitening agent,<sup>42</sup> skin whitening agent,<sup>43</sup> wound healing promoter<sup>44</sup>

**Safety/Toxicity** Carcinogenicity,<sup>45</sup> cell toxicity,<sup>46</sup> ecotoxicity,<sup>47</sup> effects on breast feeding,<sup>48</sup> effects on children during pregnancy,<sup>49</sup> genotoxicity,<sup>50</sup> hepatotoxicity,<sup>51</sup> in vitro toxicity,<sup>52</sup> mutagenicity,<sup>53</sup> neurotoxicity<sup>54</sup>

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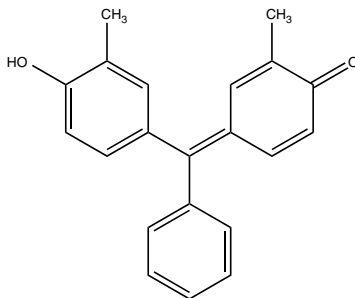
**o-CRESOLBENZEIN**

**Other Names** 2,5-Cyclohexadien-1-one, 4-(4-hydroxy-3-methyl- $\alpha$ -phenylbenzylidene)-2-methyl-;  
o-Cresolbenzein

**CA Index Name** 2,5-Cyclohexadien-1-one, 4-[(4-hydroxy-3-methylphenyl)-phenylmethylene]-2-methyl-

**CAS Registry Number** 5664-07-3

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Benzein

**Molecular Formula**  $C_{21}H_{18}O_2$

**Molecular Weight:** 302.37

**pH Range** 7.2–8.6

**Color Change at pH** Yellow (7.2) to red (8.6)

**pKa** 9.66

**Physical Form** Red-orange crystals

**Solubility** Insoluble in water; soluble in ethanol

**Melting Point** 260–262°C

**Boiling Point (Calcd.)**  $505.4 \pm 50.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Cosmetics<sup>3</sup>

**Safety/Toxicity** No data available

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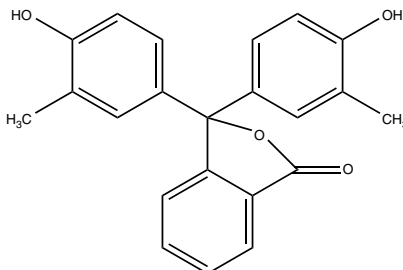
**o-CRESOLPHTHALEIN**

**Other Names** Phenolphthalein, 3',3''-dimethyl-; o-Cresolphthalein; 3,3-Bis(3-methyl-4-hydroxyphenyl)phthalide; Cresolphthalein

**CA Index Name** 1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxy-3-methylphenyl)-

**CAS Registry Number** 596-27-0

**Merck Index Number** 2576

**Chemical Structure**

**Chemical/Dye Class** Phthalein

**Molecular Formula** C<sub>22</sub>H<sub>18</sub>O<sub>4</sub>

**Molecular Weight** 346.38

**pH Range** 8.2–9.8

**Color Change at pH** Colorless (8.2) to red (9.8)

**pKa** 9.40

**Physical Form** Buff or beige powder

**Solubility** Slightly soluble in water; soluble in ethanol

**UV-Visible (λ<sub>max</sub>)** 566 nm, 381 nm

**Melting Point** 223°C

**Boiling Point (Calcd.)** 555.0 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–8</sup>

**Major Applications** Sensors,<sup>9–11</sup> display device,<sup>12</sup> photoresists,<sup>13</sup> recording materials,<sup>14</sup> imaging materials,<sup>15</sup> authentication system for secure documents,<sup>16</sup> decoder system,<sup>17</sup> lithium cells,<sup>18</sup> electroplating process,<sup>19</sup> inks,<sup>20,21</sup> markers,<sup>22</sup> toners,<sup>23</sup> correction fluid,<sup>24</sup> paints,<sup>25</sup> adhesives,<sup>26,27</sup> floor coatings,<sup>28</sup> gas leaking detector for safety in industries,<sup>29</sup> toys,<sup>30</sup> food storage,<sup>31</sup> diapers,<sup>32</sup> determination of calcium,<sup>33</sup> lotions,<sup>34</sup> urine analysis test strips,<sup>35</sup> drugs,<sup>36</sup> blood analysis<sup>37</sup>

**Safety/Toxicity** Toxic effects to health and environments<sup>38</sup>

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## o-CRESOLPHTHALEIN COMPLEXON

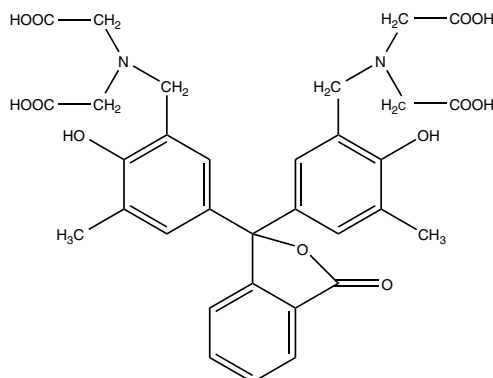
**Other Names** Phenolphthalein, 3',3''-bis[[bis(carboxymethyl)amino]methyl]-5',5''-dimethyl-; 3,3'-Bis[*N,N*-bis(carboxymethyl)aminomethyl]-*o*-cresolphthalein; 3,3'-Bis[*N,N*-di(carboxymethyl)aminomethyl]-*o*-cresolphthalein; Cresolphthalein complexon; Cresolphthalexon; NSC 298195; Phthalein complexone; *o*-Cresolphthalein complexon; *o*-Cresolphthalein complexone; *o*-Cresolphthalexon; *o*-Cresolphthalexone; Metalphthalein; Phthalein Purple

**CA Index Name** Glycine, *N,N'*-[(3-oxo-1(3H)-isobenzofuranylidene)bis[(6-hydroxy-5-methyl-3,1-phenylene)methylene]]bis[*N*-(carboxymethyl)-

**CAS Registry Number** 2411-89-4

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Phthalein

**Molecular Formula** C<sub>32</sub>H<sub>32</sub>N<sub>2</sub>O<sub>12</sub>

**Molecular Weight** 636.60

**pH Range** 8.2–9.8

**Color Change at pH** Colorless (8.2) to red (9.8)

**pKa** 1.47, 8.24

**Physical Form** Light pink powder

**Solubility** Soluble in water, ethanol

**UV-Visible (λ<sub>max</sub>)** 575 nm, 377 nm

**Melting Point** 181–185°C

**Boiling Point (Calcd.)** 892.1 ± 65.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–6</sup>

**Major Applications** Sensors,<sup>7–10</sup> photoconductors,<sup>11</sup> copying materials,<sup>12</sup> rubber,<sup>13–15</sup> body fluid testing,<sup>16</sup> determination of calcium,<sup>17</sup> magnesium,<sup>18</sup> tin,<sup>19</sup> method for measuring urea nitrogen,<sup>20</sup> liposomal construct for diagnostic use,<sup>21</sup> cardiovascular disease,<sup>22</sup> antibacterial agent<sup>23</sup>

**Safety/Toxicity** *In vitro* toxicity<sup>23</sup>

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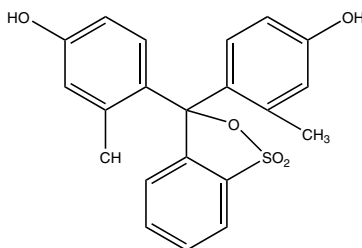
***m*-CRESOL PURPLE**

**Other Names** Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[3-methyl-, *S,S*-dioxide; *m*-Cresol purple; *m*-Cresol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)di-, *S,S*-dioxide; *o*-Toluenesulfonic acid,  $\alpha$ -hydroxy- $\alpha,\alpha$ -bis(4-hydroxy-*o*-tolyl)-,  $\gamma$ -sultone; 3H-2,1-Benzoxathiole, phenol derivative; Cresol purple; Metacresol Purple; NSC 9607; *m*-Cresolsulfonephthalein

**CA Index Name:** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[3-methyl-

**CAS Registry Number:** 2303-01-7

**Merck Index Number** 2577

**Chemical Structure**

**Chemical/Dye Class:** Sulfonephthalein

**Molecular Formula:** C<sub>21</sub>H<sub>18</sub>O<sub>5</sub>S

**Molecular Weight:** 382.43

**pH Range** 1.2–2.8;

7.4–9.0

**Color Change at pH** Red (1.2) to yellow (2.8)

Yellow (7.4) to purple (9.0)

**pKa** 1.51, 8.32

**Physical Form** Dark brown glittering crystals or olive green powder

**Solubility** Very slightly soluble in water, ethanol; soluble in methanol

**UV-Visible ( $\lambda_{\text{max}}$ )** 579 nm, 371 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 577.5  $\pm$  50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Fuel cells,<sup>6</sup> sensors,<sup>7</sup> display device,<sup>8</sup> falsification-proof security paper,<sup>9</sup> inks,<sup>10</sup> correction fluid,<sup>11</sup> paints,<sup>12</sup> detection of electrophilic gases,<sup>13</sup> lubricants,<sup>14</sup> cement products,<sup>15</sup> packaging system,<sup>16</sup> adhesive,<sup>17</sup> cosmetics,<sup>18</sup> food storage,<sup>19</sup> determining glucose in dialysis solution,<sup>20</sup> screening of cat diseases,<sup>21</sup> detecting carbohydrates,<sup>22</sup> oral hygiene products<sup>23</sup>

**Safety/Toxicity** No data available

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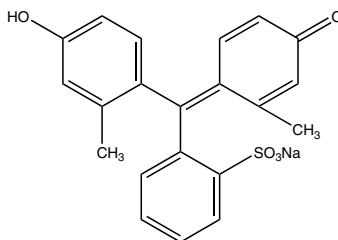
**m-CRESOL PURPLE, SODIUM SALT**

**Other Names** Phenol, 4,4'-(3H-1,2-benzoxathiol-3-ylidene)bis[3-methyl-, S,S-dioxide, monosodium salt; 3H-1,2-Benzoxathiole, phenol derivative

**CA Index Name** Phenol, 4,4'-(2,2-dioxido-3H-1,2-benzoxathiol-3-ylidene)bis[3-methyl-, monosodium salt

**CAS Registry Number** 62625-31-4

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class:** Sulfonephthalein

**Molecular Formula** C<sub>21</sub>H<sub>17</sub>O<sub>5</sub>SNa

**Molecular Weight** 404.42

**pH Range** 1.2–2.8

7.4–9.0

**Color Change at pH** Red (1.2) to yellow (2.8)

Yellow (7.4) to purple (9.0)

**pKa** 1.51, 8.32

**Physical Form** Black powder

**Solubility** Soluble in water, ethanol

**UV-Visible (λ<sub>max</sub>)** 436 nm

**Melting Point** >250°C

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Screening method of endocrine disrupting chemicals<sup>2</sup>

**Safety/Toxicity** No data available

**References**

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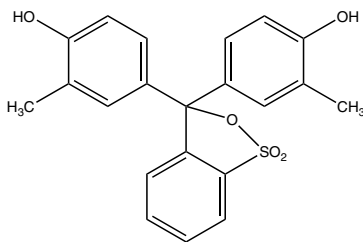
**o-CRESOL RED**

**Other Names** Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-methyl-, *S,S*-dioxide; *o*-Cresol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)di-, *S,S*-dioxide; *o*-Cresolsulfonephthalein; *o*-Toluenesulfonic acid,  $\alpha$ -hydroxy- $\alpha,\alpha$ -bis(4-hydroxy-*m*-tolyl)-,  $\gamma$ -sultone; 3H-2,1-Benzoxathiole, phenol derivative; 3',3''-Dimethylphenolsulfonephthalein; Cresol red; Cresolsulfophthalein; NSC 7224; *o*-Cresol Red; *o*-Cresolsulfonphthalein

**CA Index Name:** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-methyl-

**CAS Registry Number:** 1733-12-6

**Merck Index Number** 2578

**Chemical Structure**

**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula**  $C_{21}H_{18}O_5S$

**Molecular Weight** 382.43

**pH Range** 0.2–1.8

7.0–8.8

**Color Change at pH** Red (0.2) to yellow (1.8)

Yellow (7.0) to reddish-purple (8.8)

**pKa** 1.4, 8.2, 8.3

**Physical Form** Green glittering crystals or reddish-brown powder

**Solubility** Sparingly soluble in water; soluble in ethanol

**UV-Visible ( $\lambda_{max}$ )** 570 nm, 367 nm, 432 nm

**Melting Point** >300°C

**Boiling Point (Calcd.)**  $561.9 \pm 50.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Display device,<sup>6</sup> optical sensors,<sup>7</sup> combustion gas detection system,<sup>8</sup> inks,<sup>9</sup> correction fluid,<sup>10</sup> diapers,<sup>11</sup> toothpaste,<sup>12</sup> identifying fresh and stale rice,<sup>13</sup> food storage,<sup>14</sup> determine glucose in dialysis solution,<sup>15</sup> monitor metabolic activity of microorganisms,<sup>16</sup> detect bacterial infection,<sup>17</sup> psychoactive drugs,<sup>18</sup> dental impression material<sup>19</sup>

**Safety/Toxicity** No data available

**References**

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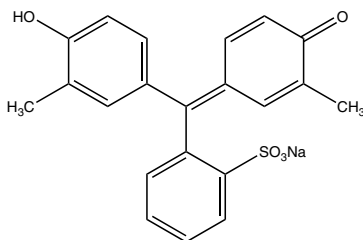
**o-CRESOL RED, SODIUM SALT**

**Other Names** Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-methyl-, S,S-dioxide, monosodium salt; 3H-2,1-Benzoxathiole, phenol derivative

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-methyl-, monosodium salt

**CAS Registry Number** 62625-29-0

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>21</sub>H<sub>17</sub>O<sub>5</sub>SNa

**Molecular Weight** 404.42

**pH Range** 0.2–1.8

7.0–8.8

**Color Change at pH** Red (0.2) to yellow (1.8)

Yellow (7.0) to reddish-purple (8.8)

**pKa** 1.4, 8.2, 8.3

**Physical Form** Brown powder

**Solubility** Soluble in water, ethanol

**UV-Visible (λ<sub>max</sub>)** 425 nm

**Melting Point** 250°C (decompose)

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Thermochromic materials,<sup>2</sup> cosmetics,<sup>1</sup> measurement of hydrophobicity of therapeutic drugs<sup>3</sup>

**Safety/Toxicity** No data available

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## CRYSTAL VIOLET

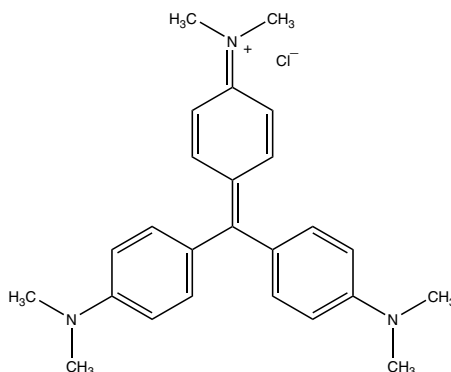
**Other Names** C.I. Basic Violet 3; 12416 Violet; Adergon; Aizen Crystal Violet; Aizen Crystal Violet Extra Pure; Aniline violet; Aniline violet pyoktanine; Atmonil; Avermin; Axuris; Badil; Basic Violet 3; Basic Violet BN; Basonyl Violet 610; C.I. 42555; Calcozine Violet 6BN; Calcozine Violet C; Crystal Violet 10B; Crystal Violet 5BO; Crystal Violet 6B; Crystal Violet 6BO; Crystal Violet AO; Crystal Violet AON; Crystal Violet BP; Crystal Violet BPC; Crystal Violet Extra Pure; Crystal Violet Extra Pure APN; Crystal Violet Extra Pure APNX; Crystal Violet FN; Crystal Violet HL 2; Crystal Violet O; Crystal Violet Pure DSC; Crystal Violet Pure DSC Brilliant; Crystal Violet SS; Crystal Violet Technical; Crystal Violet USP; Crystal Violet chloride; Crystal violet; Gentsal; Gentian Violet B; Gentian violet; Gentiaverm; Gentacid; Gentioletten; Hecto Violet R; Hectograph Violet SR; Hexamethyl violet; Hexamethyl-*p*-rosaniline chloride; Hexamethylpararosaniline chloride; Hidaco Brilliant Crystal Violet; Meroxyl; Meroxyl-Wander; Meroxylan; Meroxylan-Wander; Methyl Violet 10B; Methyl Violet 10BD; Methyl Violet 10BK; Methyl Violet 10BN; Methyl Violet 10BNS; Methyl Violet 10BO; Methyl Violet 5BNO; Methyl Violet 5BO; Methyl Violet 6B; Methyl Violet 6B (biological stain); Methylrosaniline chloride; Methylrosanilinium chloride; Mitsui Crystal Violet; Oxiuran; Oxycolor; Oxyozyl; Paper Blue R; Pararosaniline, *N,N,N',N',N'',N''*-hexamethyl-, chloride; Plastoresin Violet 5BO; Pyoktanin; Sanyo Fanal Violet R; Vermicid; Vianin; Viocid; Violet 5BO; Violet 6BN; Violet CP; Violet XXIII; crystal violet

**CA Index Name** Methanaminium, *N*-[4-*bis*[4-(dimethylamino)phenyl]methylene]-2,5-cyclohexadien-1-ylidene]-*N*-methyl-, chloride

**CAS Registry Number** 548-62-9

**Merck Index Number** 4395

### Chemical Structure



**Chemical/Dye Class** Triphenylmethane

**Molecular Formula**  $C_{25}H_{30}N_3Cl$

**Molecular Weight** 407.99

**pH Range** 0.0–2.0

**Color Change at pH** Yellow (0.0) to blue-violet (2.0)

**pKa** 9.4

**Physical Form** Green to yellowish-green powder

**Solubility** Soluble in water, acetone, chloroform; very soluble in ethanol; practically insoluble in ether; insoluble in xylene

**UV-Visible ( $\lambda_{max}$ )** 590 nm

**Melting Point** 205–215°C (decompose)

**Synthesis** Synthetic methods<sup>1–12</sup>

**Major Applications** Photoresists,<sup>13</sup> lithographic printing plate,<sup>14</sup> printed circuit board,<sup>15</sup> inks,<sup>16</sup> detergent,<sup>17</sup> hair dyes,<sup>18</sup> shampoo,<sup>19</sup> drug screening method,<sup>20</sup> bone cement preparation method,<sup>21</sup> treating microorganisms,<sup>22</sup> hemorrhoids,<sup>23</sup> antifungal,<sup>24</sup> antibacterial,<sup>25</sup> antimalarial agent,<sup>26</sup> dental application<sup>27</sup>

**Safety/Toxicity** Acute oral toxicity,<sup>28</sup> chronic toxicity,<sup>29,30</sup> carcinogenicity,<sup>29,30</sup> cytotoxicity,<sup>31</sup> genotoxicity,<sup>32</sup> mutagenicity,<sup>33,34</sup> ototoxicity,<sup>35</sup> percutaneous toxicity,<sup>36</sup> phototoxicity<sup>37</sup>

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## CURCUMIN

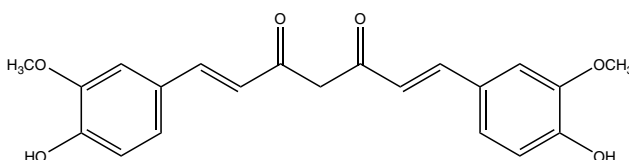
**Other Names** 1,6-Heptadiene-3,5-dione, 1,7-bis(4-hydroxy-3-methoxyphenyl)-, (E,E)-; Curcumin; (E,E)-1,7-Bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione; C Yellow 15; C.I. 75300; C.I. Natural Yellow 3; Curcuma; Curcumin I; Curcumine; Diferuloylmethane; E 100; E 100 (dye); Haidr; Halad; Haldar; Halud; Indian Saffron; Kacha Haldi; Merita Earth; NSC 32982; Natural Yellow 3; San-Ei Curcumine AL; San-Ei Gen Curcumine AL; Souchet; Terra Merita; Turmeric; Turmeric (dye); Turmeric yellow; Ukon; Ukon (dye); Yellow Ginger; Yellow Root; Yo-Kin; trans,trans-Curcumin

**CA Index Name** 1,6-Heptadiene-3,5-dione, 1,7-bis(4-hydroxy-3-methoxyphenyl)-, (1E,6E)-

**CAS Registry Number** 458-37-7

**Merck Index Number** 2673

### Chemical Structure



**Chemical/Dye Class** Miscellaneous, Chalcone

**Molecular Formula** C<sub>21</sub>H<sub>20</sub>O<sub>6</sub>

**Molecular Weight** 368.38

**pH Range** 7.8–9.2

**Color Change at pH** Yellow (7.8) to red-brown (9.2)

**pKa** 8.09

**Physical Form** Orange-yellow crystalline powder

**Solubility** Insoluble in water, ether; soluble in ethanol, acetic acid, dimethyl sulfoxide

**UV-Visible (λ<sub>max</sub>)** 430 nm

**Melting Point** 183°C

**Boiling Point (Calcd.)** 591.4 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–7</sup>

**Major Applications** Cosmetics,<sup>8</sup> drug-eluting stents,<sup>9</sup> inhibition of formation of skin-wrinkles,<sup>10</sup> treating alzheimer's disease,<sup>11</sup> skin diseases,<sup>12</sup> coronary restenosis,<sup>13</sup> diabetes,<sup>14</sup> obesity,<sup>14</sup> leukemia,<sup>15</sup> neurofibromas,<sup>16</sup> cancer,<sup>17</sup> antimicrobial,<sup>18</sup> antiviral,<sup>19</sup> antiinflammatory,<sup>20</sup> antiprostata cancer<sup>21</sup>

**Safety/Toxicity** Mitochondrial and DNA damage,<sup>22</sup> chronic toxicity,<sup>23</sup> tissue-specific toxicity,<sup>24</sup> carcinogenicity,<sup>25,26</sup> cytotoxicity,<sup>27</sup> excitotoxicity,<sup>28</sup> hepatotoxicity,<sup>29</sup> oral toxicity,<sup>30</sup> mutagenicity<sup>31</sup>

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# D

## DICHLOROFLUORESCEIN

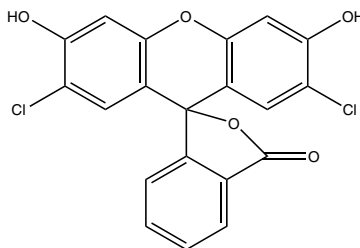
**Other Names** Fluorescein, 2',7'-dichloro-; 2',7'-Dichlorofluorescein; D and C Orange 25; D and C Orange No. 25; Fluorescein 27; Fluorescein 548

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 2',7'-dichloro-3',6'-dihydroxy-

**CAS Registry Number** 76-54-0

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>20</sub>H<sub>10</sub>Cl<sub>2</sub>O<sub>5</sub>

**Molecular Weight** 401.20

**pH Range** 4.0–6.0

**Color Change at pH** Weak green fluorescence (4.0) to intense green fluorescence (6.0)

**pKa** 4.46

**Physical Form** Light orange powder

**Solubility** Insoluble in water; soluble in ethanol; slightly soluble in ether, methanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 509 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 634.4 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Electroluminescent devices,<sup>3</sup> sol-gel silica films,<sup>4</sup> integrated circuits,<sup>5</sup> photoresists,<sup>6</sup> recording material,<sup>7</sup> LED devices,<sup>8</sup> photoconductors,<sup>9</sup> Solid-state dye laser,<sup>10</sup> lithographic printing plates,<sup>11</sup> inks,<sup>12</sup> Fluorescent pH sensors,<sup>13</sup> emissive probes,<sup>14</sup> chemotherapeutic treatment of disease,<sup>15</sup> phototherapeutic treatment of disease,<sup>16</sup> photodynamic treatment of disease<sup>17</sup>

**Safety/Toxicity** Carcinogenicity,<sup>18</sup> cytotoxicity,<sup>19</sup> genotoxicity,<sup>20</sup> hemoglobin toxicity,<sup>21</sup> neurotoxicity,<sup>22</sup> phototoxicity.<sup>23</sup>

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## 6,7-DIHYDROXYCOUMARIN

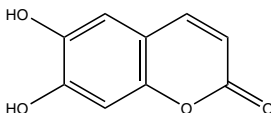
**Other Names** Coumarin, 6,7-dihydroxy-; Esculetin; 6,7-Dihydroxy-2-benzopyrone; 6,7-Dihydroxycoumarin; Aesculetin; Asculetine; Cichorigenin; Cichoriin aglycon; Esculetol; Esculin aglycon; NSC 26428; Esculetin

**CA Index Name** 2H-1-Benzopyran-2-one, 6,7-dihydroxy-

**CAS Registry Number** 305-01-1

**Merck Index Number** 3697

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Coumarin

**Molecular Formula** C<sub>9</sub>H<sub>6</sub>O<sub>4</sub>

**Molecular Weight** 178.14

**pH Range** 1.5–2.0

**Color Change at pH** Weak blue fluorescence (1.5) to strong blue fluorescence (2.0)

**pKa** 1.71

**Physical Form** Light yellow powder

**Solubility** Almost insoluble in boiling water, ether; soluble in hot ethanol, glacial acetic acid

**Melting Point** 272–274°C

**Boiling Point (Calcd.)** 469.7 ± 45.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–10</sup>

**Major Applications** Herbicides,<sup>11</sup> cosmetics,<sup>12</sup> teeth whitening agent,<sup>13</sup> antiinflammatory,<sup>14</sup> antifungal,<sup>15</sup> antibacterial,<sup>15</sup> antiviral,<sup>16</sup> treating drug-induced weight gain,<sup>17</sup> neurodegenerative and blood coagulation disorders,<sup>18</sup> cancer,<sup>19</sup> amyloidosis,<sup>20</sup> skin impairments and baldness<sup>21</sup>

**Safety/Toxicity** Cytotoxicity,<sup>22</sup> mutagenicity<sup>23</sup>

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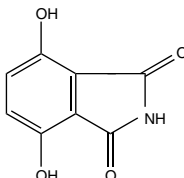
**3,6-DIHYDROXYPHTHALIMIDE**

**Other Names** Phthalimide, 3,6-dihydroxy-; 3,6-Dihydroxyphthalimide; NSC 229301

**CA Index Name** 1H-Isoindole-1,3(2H)-dione, 4,7-dihydroxy-

**CAS Registry Number** 51674-11-4

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>8</sub>H<sub>5</sub>NO<sub>4</sub>

**Molecular Weight** 179.13

**pH Range** 0.0–2.4;  
6.0–8.0

**Color Change at pH** Blue fluorescence (0.0) to green fluorescence (2.4)

Green fluorescence (6.0) to yellow/green fluorescence (8.0)

**pKa** 1.65, 6.97

**Physical Form** White solid

**Solubility** Insoluble in water; soluble in ethanol, methanol

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1–4</sup>

**Major Applications** Dye lasers,<sup>5</sup> immunomodulatory assays<sup>6</sup>

**Safety/Toxicity** No data available

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## 4-DIMETHYLAMINO-2-METHYLAZOBENZENE

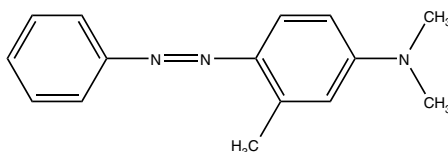
**Other Names** *m*-Toluidine, *N,N*-dimethyl-4-(phenylazo)-; 2-MeDAB; 2-Methyl-4-(dimethylamino) azobenzene; 4-(Dimethylamino)-2-methylazobenzene; 4-(*N,N*-Dimethylamino)-2-methylazobenzene; *N,N*-Dimethyl-4-(phenylazo)-*m*-toluidine; NSC 102372

**CA Index Name** Benzenamine, *N,N*,3-trimethyl-4-(phenylazo)-

**CAS Registry Number** 54-88-6

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>15</sub>H<sub>17</sub>N<sub>3</sub>

**Molecular Weight** 239.32

**pH Range** 2.8–4.4

**Color Change at pH** Red (2.8) to yellow (4.4)

**pKa** 3.68

**Physical Form** Red-orange crystals

**Solubility** Practically insoluble in water; soluble in ethanol, acetone

**UV-Visible (λ<sub>max</sub>)** 420 nm

**Melting Point** 67–69°C

**Boiling Point (Calcd.)** 390.9 ± 35.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Nematocides,<sup>3,4</sup> as diagnostic agent for diseases related with amyloid accumulation,<sup>5</sup> hepatocarcinogenesis<sup>6</sup>

**Safety/Toxicity** Carcinogenicity,<sup>7–13</sup> mutagenicity,<sup>14–22</sup> chromosome aberration,<sup>23</sup> cytotoxicity<sup>24</sup>

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## DINITROCRESOL

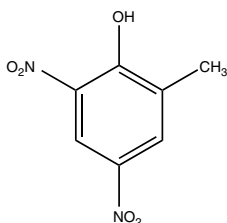
**Other Names** *o*-Cresol, 4,6-dinitro-; 2,4-Dinitro-6-methylphenol; 2-Methyl-4,6-dinitrophenol; 3,5-Dinitro-2-hydroxytoluene; 4,6-Dinitro-2-methylphenol; 4,6-Dinitro-*o*-cresol; 6-Methyl-2,4-dinitrophenol; Antinonin; Antinonnin; Arborol; DNOC; Degrasan; Dekrysil; Detal; Dillex; Dinitro; Dinitro-*o*-cresol; Dinitrocresol; Dinitrodendtroxal; Dinitrol; Dinoc; Dinurania; Ditrosol; Effusan; Effusan 3436; Elgetol; Elgetol 30; Elipol; Extrar; Flavin-Sandoz; Hedolit; Hedolite; K III; K IV; Kreozan; Krezotol 50; Lipan; NSC 2082; Neudorff DN 50; Nitrofan; Prokarbol; Rafex; Rafex 35; Raphatox; Sandolin; Sandolin A; Selinon; Sinox; Winterwash

**CA Index Name** Phenol, 2-methyl-4,6-dinitro-

**CAS Registry Number** 534-52-1

**Merck Index Number** 3279

### Chemical Structure



**Chemical/Dye Class** Nitro

**Molecular Formula**  $C_7H_6N_2O_5$

**Molecular Weight** 198.13

**pH Range** 2.4–3.8

**Color Change at pH** Colorless (2.4) to yellow (3.8)

**pKa** 4.42

**Physical Form** Yellow prisms

**Solubility** Sparingly soluble in water; readily soluble in ethanol, acetone, ether

**Melting Point** 87.5°C

**Boiling Point** 378°C

**Synthesis** Synthetic methods<sup>1–8</sup>

**Major Applications** Explosives,<sup>9</sup> fungicides,<sup>10</sup> herbicides,<sup>11,12</sup> insecticides,<sup>13,14</sup> pesticides,<sup>15,16</sup> anti-tumor agent,<sup>17</sup>

**Safety/Toxicity** Acute toxicity,<sup>18</sup> aquatic toxicity,<sup>19</sup> ecotoxicity,<sup>20</sup> environmental pollutants,<sup>21</sup> mutagenicity,<sup>22</sup> spermatotoxic effects<sup>23</sup>

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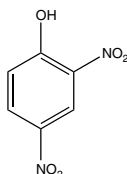
**$\alpha$ -DINITROPHENOL**

**Other Names**  $\alpha$ -Dinitrophenol; 1-Hydroxy-2,4-dinitrobenzene; 2,4-DNP; 2,4-Dinitrophenol; Aldifen; DNP; Dinitrophenol; Dinofan; Fenoxyl Carbon N; NSC 1532; Nitrophen; Nitrophen; Phenol,  $\alpha$ -dinitro-

**CA Index Name** Phenol, 2,4-dinitro-

**CAS Registry Number** 51-28-5

**Merck Index Number** 3280

**Chemical Structure**

**Chemical/Dye Class** Nitro

**Molecular Formula**  $C_6H_4N_2O_5$

**Molecular Weight** 184.11

**pH Range** 2.0–4.7

**Color Change at pH** Colorless (2.0) to yellow (4.7)

**pKa** 3.8, 3.9, 4.0, 4.1

**Physical Form** Light yellow crystals

**Solubility** Sparingly soluble in water; soluble in ethanol, benzene

**Melting Point** 112–114°C

**Boiling Point (Calcd.)**  $312.1 \pm 27.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–10</sup>

**Major Applications** Display device,<sup>11</sup> recording materials,<sup>12</sup> inks,<sup>13</sup> paints,<sup>14</sup> method for preserving food,<sup>15</sup> method for gene expression profiling,<sup>16</sup> treatment of parasitic diseases,<sup>17</sup> neurological diseases,<sup>18</sup> epilepsy,<sup>19</sup> cancer,<sup>20–22</sup> keratin materials,<sup>23</sup> neoplasms,<sup>24</sup> infectious diseases,<sup>25</sup> neutropenia,<sup>26</sup> detecting chromosome aberrations,<sup>27</sup> bacteria in gastrointestinal track<sup>28</sup>

**Safety/Toxicity** Acute toxicity,<sup>29</sup> ecotoxicity,<sup>30</sup> cytotoxicity,<sup>31</sup> environmental toxicity,<sup>32</sup> genotoxicity<sup>33</sup>

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**$\beta$ -DINITROPHENOL**

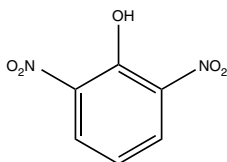
**Other Names**  $\beta$ -Dinitrophenol; 2,6-DNP; 2,6-Dinitrophenol; NSC 6215; Phenol,  $\beta$ -dinitro-; *o*-Dinitrophenol

**CA Index Name** Phenol, 2,6-dinitro-

**CAS Registry Number** 573-56-8

**Merck Index Number** 3282

**Chemical Structure**



D

**Chemical/Dye Class** Nitro

**Molecular Formula**  $C_6H_4N_2O_5$

**Molecular Weight** 184.11

**pH Range** 1.7–4.4

**Color Change at pH** Colorless (1.7) to yellow (4.4)

**pKa** 3.69, 3.7, 3.5

**Physical Form** Yellowish crystals

**Solubility** Sparingly soluble in water; soluble in ethanol, chloroform, ether

**Melting Point** 63–64°C

**Boiling Point (Calcd.)** 239.0  $\pm$  20.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–7</sup>

**Major Applications** Energetic materials,<sup>8</sup> battery,<sup>9</sup> lubricants,<sup>10</sup> curing agents for epoxy resins,<sup>11</sup> fungicidal,<sup>12</sup> herbicidal,<sup>13</sup> food storage,<sup>14</sup> drugs<sup>15</sup>

**Safety/Toxicity** Ecotoxicity,<sup>16</sup> acute toxicity,<sup>17</sup> mutagenicity<sup>18</sup>

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## $\gamma$ -DINITROPHENOL

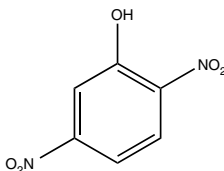
**Other Name** 2,5-DNP; 2,5-Dinitrophenol; NSC 90441; Phenol,  $\gamma$ -dinitro-

**CA Index Name** Phenol, 2,5-dinitro-

**CAS Registry Number** 329-71-5

**Merck Index Number** 3281

**Chemical Structure**



**Chemical/Dye Class** Nitro

**Molecular Formula**  $C_6H_4N_2O_5$

**Molecular Weight** 184.11

**pH Range** 4.0–5.8

**Color Change at pH** Colorless (4.0) to yellow (5.8)

**pKa** 5.21, 5.1, 5.0

**Physical Form** Yellowish needles

**Solubility** Sparingly soluble in water; soluble in ethanol, ether

**Melting Point** 108°C

**Boiling Point (Calcd.)**  $309.6 \pm 27.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–6</sup>

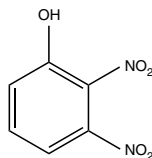
**Major Applications** Liquid crystal films,<sup>7</sup> electrophotographic materials,<sup>8</sup> adhesives,<sup>9</sup> inks,<sup>10</sup> lubricants,<sup>11</sup> preservation of cut flowers,<sup>12,13</sup> food storage,<sup>14</sup> materials for evaluating dental caries activity<sup>15</sup>

**Safety/Toxicity** Aquatic toxicity,<sup>16</sup> cytotoxicity,<sup>17</sup> ecotoxicity,<sup>18</sup> environmental toxicity<sup>19</sup>

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**$\epsilon$ -DINITROPHENOL****Other Names** 2,3-DNP; 2,3-Dinitrophenol; NSC 156083**CA Index Name** Phenol, 2,3-dinitro-**CAS Registry Number** 66-56-8**Merck Index Number** Not listed**Chemical Structur****D****Chemical/Dye Class** Nitro**Molecular Formula**  $C_6H_4N_2O_5$ **Molecular Weight** 184.11**pH Range** 3.9–5.9**Color Change at pH** Colorless (3.9) to yellow (5.9)**pKa** 4.86, 4.96**Physical Form** Yellow needles**Solubility** Sparingly soluble in water; soluble in ethanol, ether**Melting Point** 145°C**Boiling Point (Calcd.)**  $328.9 \pm 27.0^\circ\text{C}$  Pressure: 760 Torr**Synthesis** Synthetic methods<sup>1–5</sup>**Major Applications** For biosensor design,<sup>6</sup> drug delivery<sup>7</sup>**Safety/Toxicity** Toxicity,<sup>8</sup> toxicology,<sup>9</sup> ecotoxicity,<sup>10</sup> toxic actions,<sup>11</sup> mutagenicity<sup>12</sup>**References**

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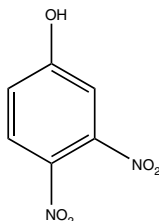
**$\delta$ -DINITROPHENOL**

**Other Names** 3,4-DNP; 3,4-Dinitrophenol; 6,5-Dinitrophenol; Phenol,  $\delta$ -dinitro-

**CA Index Name** Phenol, 3,4-dinitro-

**CAS Registry Number** 577-71-9

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Nitro

**Molecular Formula**  $C_6H_4N_2O_5$

**Molecular Weight** 184.11

**pH Range** 4.3–6.3

**Color Change at pH** Colorless (4.3) to yellow (6.3)

**pKa** 5.35, 5.42

**Physical Form** Light yellow needles

**Solubility** Sparingly soluble in water; soluble in ethanol, ether

**Melting Point** 134°C

**Boiling Point (Calcd.)**  $418.7 \pm 35.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Lubricants,<sup>6</sup> enzyme assay,<sup>7</sup> antinerve agent,<sup>8</sup> substrate for enzymes,<sup>9</sup> in biotechnological process,<sup>10</sup> for biosensor design<sup>11</sup>

**Safety/Toxicity** Toxicity,<sup>12,13</sup> toxicology,<sup>14</sup> ecotoxicity,<sup>15</sup> mutagenicity<sup>16</sup>

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## 2,4-DINITROPHENYLHYDRAZINE

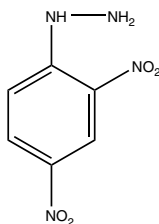
**Other Names** (2,4-Dinitrophenyl)hydrazine; 1-(2,4-Dinitrophenyl)hydrazine; 1-Hydrazino-2,4-dinitrobenzene; DNPH; NSC 5709

**CA Index Name** Hydrazine, (2,4-dinitrophenyl)-

**CAS Registry Number** 119-26-6

**Merck Index Number** 3283

### Chemical Structure



**Chemical/Dye Class** Miscellaneous

**Molecular Formula** C<sub>6</sub>H<sub>6</sub>N<sub>4</sub>O<sub>4</sub>

**Molecular Weight** 198.14

**pH Range** 11.0–12.5

**Color Change at pH** Yellow (11.0) to brown (12.5)

**pKa** 12.1

**Physical Form** Red crystals

**Solubility** Slightly soluble in water, ethanol

**Melting Point** 200°C

**Boiling Point (Calcd.)** 378.6 ± 32.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Fuel cells,<sup>3</sup> detecting microorganisms,<sup>4</sup> antibacterial agent,<sup>5</sup> treatment of acute and chronic hepatitis,<sup>6</sup> gynecopathy,<sup>7</sup> cardiovascular diseases,<sup>8</sup> cerebrovascular diseases<sup>8</sup>

**Safety/Toxicity** Bladder toxicity,<sup>9</sup> carcinogenicity,<sup>10</sup> genotoxicity,<sup>11</sup> mutagenicity<sup>12</sup>

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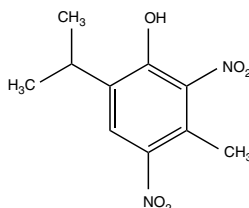
**DINITROTHYMOL**

**Other Names** Thymol, 2,6-dinitro-; 2,4-Dinitrothymol; 2,6-Dinitrothymol; 2-Isopropyl-5-methyl-4,6-dinitrophenol; NSC 6767

**CA Index Name** Phenol, 3-methyl-6-(1-methylethyl)-2,4-dinitro-

**CAS Registry Number** 303-21-9

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Nitro

**Molecular Formula** C<sub>10</sub>H<sub>12</sub>N<sub>2</sub>O<sub>5</sub>

**Molecular Weight** 240.21

**pH Range** 2.2–3.4

**Color Change at pH** Colorless (2.2) to yellow (3.4)

**pKa** 4.86

**Physical Form** Yellow crystals

**Solubility** Insoluble in water; soluble in ethanol, methanol

**Melting Point** >250°C

**Boiling Point (Calcd.)** 311.7 ± 42.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1</sup>

**Major Applications** Antileishmanial drug<sup>1</sup>

**Safety/Toxicity** Acute oral toxicity<sup>2</sup>

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**DIRECT BLUE 72**

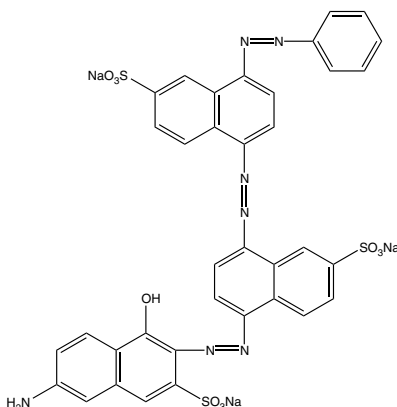
**Other Names** C.I. Direct Blue 72; C.I. 34145; Diazol Light Blue B; Direct Fast Blue FR

**CA Index Name** 2-Naphthalenesulfonic acid, 5-[[[(6-amino-1-hydroxy-3-sulfo-2-naphthalenyl)azo]-8-[[4-(phenylazo)-6-sulfo-1-naphthalenyl]azo]-, trisodium salt

**CAS Registry Number** 6717-34-6

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{36}H_{22}N_7O_{10}S_3Na_3$

**Molecular Weight** 877.76

**pH Range** 13.0–14.0

**Color Change at pH** Blue (13.0) to violet (14.0)

**pKa** 13.8

**Physical Form** Dark blue powder

**Solubility** Soluble in water, ethanol

**Melting Point**  $>300^{\circ}\text{C}$

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Coloring paper<sup>1</sup>

**Safety/Toxicity** No data available

**Reference**

1. Chekunina, L. I.; Danilova, D. A.; Polovinkin, V. L. Replacement of direct dyes during the coloring of paper. *Bumazhnaya Promyshlennost* **1975**, 15–16; *Chem. Abstr.* **1975**, 83, 149385.

## DIXYLENOLPHTHALEIN

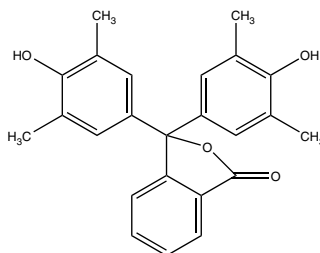
**Other Names** Phenolphthalein, 3',3'',5',5''-tetramethyl-; 2,6-Dixylenolphthalein

**CA Index Name** 1(3H)-Isobenzofuranone, 3,3-*bis*(4-hydroxy-3,5-dimethylphenyl)-

**CAS Registry Number** 3689-45-0

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Phthalein

**Molecular Formula** C<sub>24</sub>H<sub>22</sub>O<sub>4</sub>

**Molecular Weight** 374.43

**pH Range** 8.5–9.9

**Color Change at pH** Colorless (8.5) to violet (9.9)

**pKa** 9.97

**Physical Form** White powder

**Solubility** Insoluble in water; soluble in ethanol, methanol

**Melting Point** 247.5–249.0°C

**Boiling Point (Calcd.)** 556.6 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–4</sup>

**Major Applications** Indicator,<sup>4–6</sup> polymeric alloys,<sup>2</sup> toothpaste and mouthwash,<sup>7</sup> disinfectant,<sup>8</sup> cosmetics,<sup>9</sup> paints<sup>10</sup>

**Safety/Toxicity** No data available

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# E

## EOSIN Y

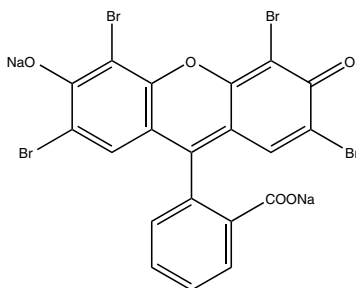
**Other Names** Eosin Yellowish; Fluorescein, 2',4',5',7'-tetrabromo-, disodium salt; 11445 Red; 11731 Red; 1903 Yellow Pink; Acid Red 87; Aizen Eosine GH; Basacid Red 316; Bromo 4D; Bromo 4DC; Bromo 4DL; Bromo B; Bromo FL; Bromo JPS; Bromo TS; Bromo X 100; Bromo XX; Bromo acid; Bromoeosine; Bromofluoresceic acid; Bromofluorescein; Bronze Bromo; C.I. 45380; C.I. Acid Red 87; Certiquel Eosine; Chugai Ink Red AM 5; D and C Red No. 22; D&C Red 22; D&C Red No. 22; Daiwa Red 103WB; Dawn red; Disodium eosin; Eosin; Eosin A; Eosin OJ; Eosin Y; Eosin YS; Eosin yellow; Eosine; Eosine 3G; Eosine 3Y; Eosine A; Eosine BPC; Eosine BS; Eosine BS-SF; Eosine DA; Eosine DWC 73; Eosine Extra Conc. A. Export; Eosine Extra Yellowish; Eosine FA; Eosine G; Eosine GF; Eosine GH; Eosine J; Eosine K; Eosine K Salt Free; Eosine Lake Red Y; Eosine OJ; Eosine S; Eosine S 13; Eosine Salt Free; Eosine Y; Eosine YB; Eosine YS; Eosine Yellow; Eosine Yellowish; Eosine sodium; Eosine sodium salt; Eosine w/s; Eosine water-soluble; Fenazo Eosine XG; Food Red 103; Hidacid Boiling Bromo; Hidacid Bromo acid regular; Hidacid Dibromo Fluorescein; Hidacid Eosine Soda Salt; Hidacid White Bromo; Irgalite Bronze Red CL; Japan Red 103; Japan Red 230-1; Japan Red 230-2; Japan Red No. 103; Japan Red No. 230-1; Morning red; Orient Water Red 2; Phlox Red Toner X 1354; Phloxine Red 20-7600; Phloxine Toner B; Pure Eosine YY; Red 103; Red No. 103; Red No. 230-1; Sodium eosin; Sodium eosinate; Sodium eosine; Symuler Eosin Toner; Tetrabromofluorescein; Tetrabromofluorescein D; Tetrabromofluorescein S; Tetrabromofluorescein soluble; Toyo Eosine G; Water Red 2

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 2',4',5',7'-tetrabromo-3',6'-dihydroxy-, disodium salt

**CAS Registry Number** 17372-87-1

**Merck Index Number** 3603

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula**  $C_{20}H_6Br_4O_5Na_2$

**Molecular Weight** 691.86

**pH Range** 0.0–3.0

**Color Change at pH** Yellow or nonfluorescence (0.0) to red or green fluorescence (3.0)

**pKa** 2.9, 4.5

**Physical Form** Red crystals

**Solubility** Freely soluble in water; slightly soluble in ethanol, methanol; insoluble in ether

**UV-Visible** ( $\lambda_{max}$ ) 514 nm

**Melting Point** 295.5°C

**Synthesis** Synthetic methods<sup>1–9</sup>

**Major Applications** Photovoltaic devices,<sup>10</sup> color filter,<sup>11</sup> nanoscale host material,<sup>12</sup> detection of latent fingerprints,<sup>13</sup> inks,<sup>14</sup> detergents,<sup>15</sup> hair dyes,<sup>16</sup> cosmetics,<sup>17</sup> implantable drug delivery devices,<sup>18</sup> stents,<sup>19</sup> diagnosis of breast lesions,<sup>20</sup> labeling nucleic acids,<sup>21</sup> detecting proteins,<sup>22</sup> stress biomarkers,<sup>23</sup> phosphoprotein,<sup>24</sup> breast cancer metastases,<sup>25</sup> antimicrobial agent,<sup>26</sup> treatment of burns,<sup>27</sup> endodontic,<sup>28</sup> diabetes,<sup>29</sup> obesity,<sup>29</sup> cancer,<sup>30</sup> radiochemotherapy,<sup>31</sup> DNA sequencing,<sup>32</sup> gene expression profiling,<sup>33</sup> wound healing promoters<sup>34,35</sup>

**Safety/Toxicity** Acute toxicity,<sup>36</sup> mutagenicity,<sup>37</sup> phototoxicity<sup>38</sup>

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## ERYTHROSIN B

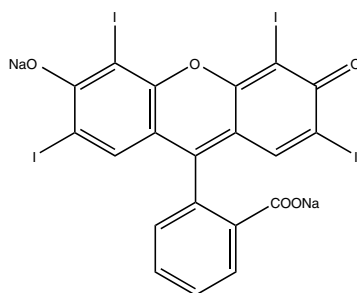
**Other Names** Fluorescein, 2',4',5',7'-tetraiodo-, disodium salt; 1427 Red; 1671 Red; 2',4',5',7'-Tetraiodofluorescein disodium salt; 2,4,5,7-Tetraiodofluorescein disodium salt; Acid Red 51; Aizen Erythrosine; Aizen Food Red 3; C.I. 45430; C.I. Acid Red 51; C.I. Food Red 14; Calco-cid Erythrosine N; Canacert Erythrosine BS; Ceplac; Cilefa Pink B; D and C Red No. 3; D&C Red No. 3; Dolkwal Erythrosine; E 127; Edicol Supra Erythrosin AS; Edicol Supra Erythrosine A; Erythrosin; Erythrosin B; Erythrosin B sodium salt; Erythrosin BS; Erythrosine; Erythrosine 3B; Erythrosine B-FO; Erythrosine BS; Erythrosine Bluish; Erythrosine Extra; Erythrosine Extra Conc. A Export; Erythrosine Extra Pure A; Erythrosine I; Erythrosine K-FO; Erythrosine TB; Erythrosine TB Extra; Erythrosine extra bluish; FD and C Red 3; FD and C Red No. 3; FD&C Red No. 3; FDC Red 3; FDC Red 3 dye; Food Color Red 3; Food Dye Red 3; Food Red 14; Food Red 3; Food Red No. 3; Hexacert Red No. 3; Hexacol Erythrosine BS; Japan Red 3; Japan Red No. 3; Maple Erythrosine; New Pink Bluish Geigy; Red 1799; S 887; Synerid; Tetraiodofluorescein sodium salt; Usacert Red No. 3

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-2',4',5',7'-tetraiodo-, disodium salt

**CAS Registry Number** 16423-68-0

**Merck Index Number** 3693

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>20</sub>H<sub>6</sub>I<sub>4</sub>O<sub>5</sub>Na<sub>2</sub>

**Molecular Weight** 879.86

**pH Range** 2.5–4.0

**Color Change at pH** Nonfluorescence (2.5) to light green or reddish fluorescence (4.0)

**pKa** 4.1

**Physical Form** Brown powder

**Solubility** Soluble in water, ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 525 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1-8</sup>

**Major Applications** Color filter,<sup>9</sup> light emitting diodes,<sup>10</sup> nanosensors,<sup>11</sup> imaging materials,<sup>12</sup> inks,<sup>13</sup> paints,<sup>14</sup> colored bubbles,<sup>15</sup> detergents,<sup>16</sup> cleaners,<sup>17</sup> cosmetics,<sup>18</sup> oral care agent,<sup>19</sup> hair dyes,<sup>20</sup> anti-septic,<sup>21</sup> treatment of burns,<sup>22</sup> diabetes,<sup>23</sup> obesity,<sup>23</sup> cancer,<sup>24</sup> viral diseases,<sup>25</sup> radiochemotherapy,<sup>26</sup> photodynamic therapy<sup>27</sup>

**Safety/Toxicity** Acute toxicity,<sup>28</sup> carcinogenicity,<sup>29</sup> cytotoxicity,<sup>30</sup> embryotoxicity,<sup>31</sup> genotoxicity,<sup>32</sup> mutagenicity,<sup>33</sup> reproductive toxicity,<sup>34</sup> neurotoxicity,<sup>34</sup> teratogenicity<sup>35</sup>

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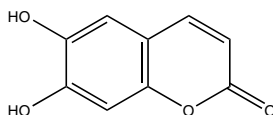
## ESCULETIN

**Other Names** Coumarin, 6,7-dihydroxy-; Esculetin; 6,7-Dihydroxy-2-benzopyrone; 6,7-Dihydroxycoumarin; Aesculetin; Aesculetine; Cichorigenin; Cichoriin aglycon; Esculetol; Esculin aglycon; NSC 26428; Esculetin

**CA Index Name** 2H-1-Benzopyran-2-one, 6,7-dihydroxy-

**CAS Registry Number** 305-01-1

**Merck Index Number** 3697

**Chemical Structure**

**Chemical/Dye Class** Fluorescent, Coumarin

**Molecular Formula** C<sub>9</sub>H<sub>6</sub>O<sub>4</sub>

**Molecular Weight** 178.14

**pH Range** 1.5–2.0

**Color Change at pH** Weak blue fluorescence (1.5) to strong blue fluorescence (2.0)

**pKa** 1.71

**Physical Form** Light yellow powder

**Solubility** Almost insoluble in boiling water, ether; soluble in hot ethanol, glacial acetic acid

**Melting Point** 272–274°C

**Boiling Point (Calcd.)** 469.7 ± 45.0 °C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–10</sup>

**Major Applications** Herbicides,<sup>11</sup> cosmetics,<sup>12</sup> teeth whitening agent,<sup>13</sup> antiinflammatory,<sup>14</sup> antifungal,<sup>15</sup> antibacterial,<sup>15</sup> antiviral,<sup>16</sup> treating drug-induced weight gain,<sup>17</sup> neurodegenerative and blood coagulation disorders,<sup>18</sup> cancer,<sup>19</sup> amyloidosis,<sup>20</sup> skin impairments and baldness<sup>21</sup>

**Safety/Toxicity** Cytotoxicity,<sup>22</sup> mutagenicity<sup>23</sup>

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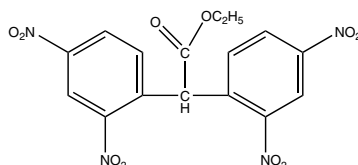
**ETHYL *BIS*-(2,4-DINITROPHENYL)ACETATE**

**Other Names** Acetic acid, *bis*(2,4-dinitrophenyl)-, ethyl ester; Ethyl *bis*(2,4-dinitrophenyl)acetate; NSC 8659; *Bis*(2,4-dinitrophenyl)-acetic acid ethyl ester

**CA Index Name** Benzeneacetic acid,  $\alpha$ -(2,4-dinitrophenyl)-2,4-dinitro-, ethyl ester

**CAS Registry Number** 5833-18-1

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Miscellaneous, Nitro

**Molecular Formula** C<sub>16</sub>H<sub>12</sub>N<sub>4</sub>O<sub>10</sub>

**Molecular Weight** 420.29

**pH Range** 7.5–9.1

**Color Change at pH** Colorless (7.5) to deep blue (9.1)

**pKa** 8.3

**Physical Form** Pale yellow crystals

**Solubility** Insoluble in water; soluble in ethanol, acetone

**Melting Point** 150–153°C

**Boiling Point (Calcd.)** 629.3 ± 55.0 °C Pressure: 760 Torr

**Synthesis** Synthetic method<sup>1,2</sup>

**Major Applications** Imaging materials,<sup>3</sup> microcapsule toner,<sup>4</sup> electrophotographic toner,<sup>5</sup> decoder system,<sup>6</sup> inks,<sup>7</sup> paints,<sup>8</sup> adhesives,<sup>9</sup> identification of organic solvents<sup>10</sup>

**Safety/Toxicity** No data available

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## ETHYL GREEN

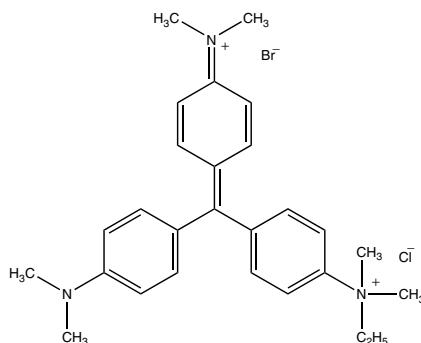
**Other Names** Ammonium, [ $\alpha$ -[*p*-(dimethylamino)phenyl]- $\alpha$ -[4-(dimethyliminio)-2,5-cyclohexadien-1-ylidene]-*p*-tolyl]-ethyl dimethyl-, bromide, chloride; [ $\alpha$ -[*p*-(Dimethylamino)-phenyl]- $\alpha$ -[4-(methyliminio)-2,5-cyclohexadien-1-ylidene]-*p*-tolyl]ethyl dimethyl ammonium bromide, methochloride; Ethyl green

**CA Index Name** Benzenaminium, 4-[[4-(dimethylamino)phenyl][4-(dimethyliminio)-2,5-cyclohexadien-1-ylidene]methyl]-*N*-ethyl-*N,N*-dimethyl-, bromide chloride

**CAS Registry Number** 14855-76-6

**Merck Index Number** 6082

**Chemical Structure**



**Note:** The traditional Methyl Green has not manufactured for decades. The dye sold as Methyl Green is more accurately described as Ethyl Green. Both, Methyl Green and Ethyl Green are sold as double zinc salts.

**Chemical/Dye Class** Triphenylmethane

**Molecular Formula**  $C_{27}H_{35}N_3BrCl$

**Molecular Weight** 516.94

**pH Range** 0.1–2.3

**Color Change at pH** Yellow (0.1) to Greenish-blue (2.3)

**Physical Form** Green power

**Solubility** Soluble in water, ethanol; insoluble in xylene

**UV-Visible ( $\lambda_{max}$ )** 635 nm, 420 nm

**Melting Point** >300°C

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Inks,<sup>2</sup> nucleic acid stain,<sup>3</sup> antifungal agent<sup>4</sup>

**Safety/Toxicity** Mutagenicity<sup>5</sup>

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## ETHYL ORANGE

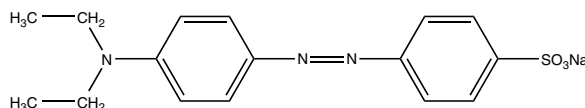
**Other Names** Benzenesulfonic acid, *p*-[[*p*-(diethylamino)phenyl]azo]-, sodium salt; Ethyl orange sodium salt; Sodium 4-[[4-(diethylamino)phenyl]azo]benzenesulfonate

**CA Index Name** Benzenesulfonic acid, 4-[[4-(diethylamino)phenyl]azo]-, sodium salt

**CAS Registry Number** 62758-12-7

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>16</sub>H<sub>18</sub>N<sub>3</sub>O<sub>3</sub>SNa

**Molecular Weight** 355.39

**pH Range** 3.4–4.8

**Color Change at pH** Red (3.4) to yellow (4.8)

**pKa** 4.34

**Physical Form** Orange powder

**Solubility** Very soluble in water; very slightly soluble in ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 474 nm

**Melting Point** >300°C

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Lithographic plate preparation,<sup>2</sup> holographic storage,<sup>3</sup> hybrid materials,<sup>4</sup> inks,<sup>5</sup> surface probes,<sup>6</sup> diagnostic agents for diseases related with amyloid accumulation<sup>7</sup>

**Safety/Toxicity** No data available

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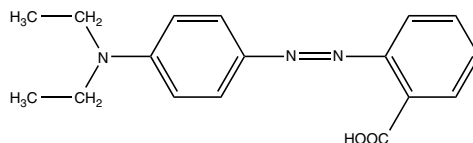
## ETHYL RED

**Other Names** 2-[4-(Diethylamino)phenylazo]benzoic acid; Ethyl Red; NSC 260474

**CA Index Name** Benzoic acid, 2-[[4-(diethylamino)phenyl]azo]-

**CAS Registry Number** 76058-33-8

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>17</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub>

**Molecular Weight** 297.35

**pH Range** 4.5–6.5

**Color Change at pH** Red (4.5) to yellow (6.5)

**pKa** 5.42

**Physical Form** Red powder

**Solubility** Almost insoluble in water; slightly soluble in ethanol, soluble in benzene

**UV-Visible** ( $\lambda_{\text{max}}$ ) 447 nm

**Melting Point** 135°C (decompose)

**Boiling Point (Calcd.)** 496.9 ± 30.0 °C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Optical materials,<sup>3–6</sup> photoresists,<sup>7,8</sup> flexible electronic circuitry,<sup>9</sup> adhesives,<sup>10</sup> textiles,<sup>11,12</sup> method for counting leukocytes,<sup>13</sup> enzyme binding assays,<sup>14</sup> DNA chips<sup>15</sup>

**Safety/Toxicity** No data available

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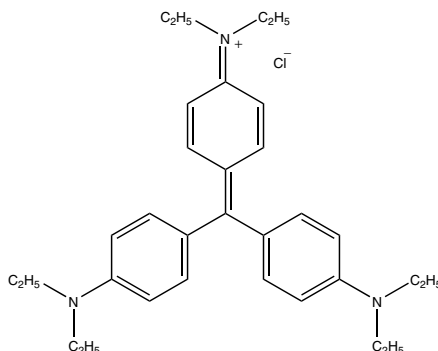
## ETHYL VIOLET

**Other Names** C.I. Basic Violet 4; Ethyl violet; Basic Violet 4; C.I. 42600; Ethyl Violet AX; Ethyl Violet GGA; Ethyl crystal violet; Lowacryl Violet 4; Shikiso Acid Brilliant Blue 6B; *Tris*(*p*-(diethylamino)-phenyl)methylm chloride

**CA Index Name** Ethanaminium, *N*-[4-[*bis*[4-(diethylamino)phenyl]methylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-, chloride

**CAS Registry Number** 2390-59-2

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Triphenylmethane

**Molecular Formula** C<sub>31</sub>H<sub>42</sub>N<sub>3</sub>Cl

**Molecular Weight** 492.15

**pH Range** 0.0–3.5

**Color Change at pH** Yellow (0.0) to blue (3.5)

**Physical Form** Olive green powder

**Solubility** Slightly soluble in water; soluble in ethanol, methanol

**UV-Visible ( $\lambda_{\text{max}}$ )** 596 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Integrated circuits,<sup>3</sup> fiber-optic pH sensors,<sup>4</sup> display device,<sup>5</sup> inks,<sup>6</sup> highlighter,<sup>7</sup> lithographic printing plates,<sup>8</sup> decoder system,<sup>9</sup> detergents,<sup>10</sup> hair dyes,<sup>11</sup> cosmetics,<sup>12</sup> wound dressing materials,<sup>13</sup> diagnosis of diseases caused by elemental imbalances,<sup>14</sup> antimicrobial,<sup>15</sup> photochemotherapeutic agent<sup>16</sup>

**Safety/Toxicity** Acute oral toxicity,<sup>17</sup> phototoxicity<sup>18</sup>

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# F

## FLUORESC EIN

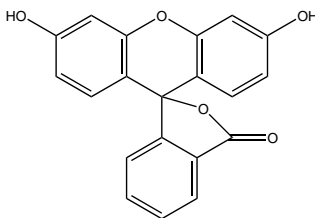
**Other Names** Fluorescein; 3',6'-Dihydroxyfluoran; 3',6'-Fluorandiol; 3,6-Dihydroxyspiro [xanthene-9,3'-phthalide]; 9-(*o*-Carboxyphenyl)-6-hydroxy-3-isoxanthenone; Benzoic acid, 2-(6-hydroxy-3-oxo-3H-xanthen-9-yl)-; C.I. 45350:1; C.I. Solvent Yellow 94; D and C Yellow No. 7; D&C Yellow No. 7; Fluorescein acid; Japan Yellow 201; Japan Yellow No. 201; NSC 667256; Resorcinolphthalein; Solvent Yellow 94; Yellow fluorescein

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-

**CAS Registry Number** 2321-07-5

**Merck Index Number** 4159

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>20</sub>H<sub>12</sub>O<sub>5</sub>

**Molecular Weight** 332.31

**pH Range** 4.0–6.0

**Color Change at pH** Pink fluorescence (4.0) to green fluorescence (6.0)

**pKa** 2.2, 4.4, 6.7

**Physical Form** Yellowish-red powder

**Solubility** Insoluble in water, ether, benzene, chloroform; soluble in ethanol, methanol, acetone, ethyl acetate, *N,N*-dimethylformamide

**UV-Visible** ( $\lambda_{\text{max}}$ ) 493.5 nm, 496 nm, 460 nm, 515 nm

**Melting Point** 315°C (decompose)

**Boiling Point (Calcd.)** 620.8 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–6</sup>

**Major Applications** Organic light-emitting diode,<sup>7</sup> nanoparticles,<sup>8</sup> liquid crystal display,<sup>9</sup> oil products,<sup>10</sup> lip make-up,<sup>11</sup> nucleic acid synthesis, amplification, sequencing and cloning,<sup>12</sup> diagnosis of diabetic retinopathy,<sup>13</sup> detecting yeast,<sup>14</sup> multidrug resistance,<sup>15</sup> proteins,<sup>16</sup> antiHCV antibodies,<sup>17</sup> target genes,<sup>18</sup> enzymatic activity,<sup>19</sup> nerve agent,<sup>20</sup> nucleic acid sequences,<sup>21</sup> imaging lung cancer,<sup>22</sup> prostate cancer<sup>23</sup>

**Safety/Toxicity** Adverse reaction,<sup>24</sup> acute toxicity,<sup>25</sup> cellular toxicity,<sup>26</sup> cytotoxicity,<sup>27</sup> mutagenicity,<sup>28</sup> phototoxicity<sup>29</sup>

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## FLUORESC EIN DIACETATE (FDA)

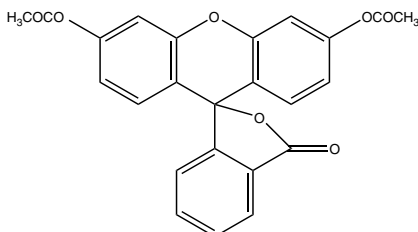
**Other Names** Fluorescein, diacetate; 3',6'-Diacetylfluorescein; Fluorescein 3',6'-diacetate; MFCD 5062; NSC 4726; NSC 667259

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-bis(acetyloxy)-

**CAS Registry Number** 596-09-8

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>24</sub>H<sub>16</sub>O<sub>7</sub>

**Molecular Weight** 416.38

**pH Range** 6.0–7.2

**Color Change at pH** Weak green fluorescence (6.0) to strong green fluorescence (7.2)

**pKa** 6.4

**Physical Form** Light yellow powder

**Solubility** Slightly soluble in water, ethanol; soluble in methanol, *N,N*-dimethylformamide

**UV-Visible ( $\lambda_{\text{max}}$ )** 490 nm

**Melting Point** 200–203°C

**Boiling Point (Calcd.)** 604.7 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** LED devices,<sup>4</sup> petroleum markers,<sup>1</sup> identifying cancerous cells,<sup>5</sup> detecting bacteria,<sup>6</sup> virus,<sup>7</sup> mitochondrial function in neurons,<sup>8</sup> target molecules,<sup>9</sup> living cells,<sup>10</sup> viable *Giardia* cysts in water samples,<sup>11</sup> apoptosis,<sup>12</sup> evaluating live/dead state of algae,<sup>13</sup> measurement of total microbial activity in soil,<sup>14</sup> treating ischemia<sup>15</sup>

**Safety/Toxicity** Cytotoxicity,<sup>16</sup> ecotoxicity,<sup>17</sup> neurotoxicity,<sup>18</sup> phytotoxicity<sup>19</sup>

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## FLUORESCEIN DISODIUM SALT

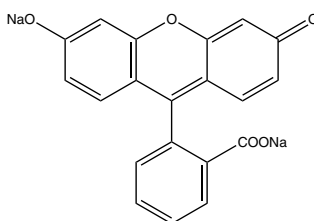
**Other Names** Fluorescein, disodium salt; Fluorin; 11824 Yellow; 12417 Yellow; 3058 Uranine; Acid Yellow 73; Aizen Uranine; Basacid Yellow 226; C.I. 45350; C.I. Acid Yellow 73; Calcocid Uranine B 4315; Certiqua Fluoresceine; D & C Yellow 8; D and C Yellow No. 8; D&C Yellow No. 8; Disodium fluorescein; Fluo-rectal; Fluor-I-Strip; Fluorescein LT; Fluorescein Sodium B.P; Fluorescein disodium; Fluorescein sodium; Fluorescein sodium salt; Fluorescite; Flurenate; Ful-Glo; Furanium; Hidacid Uranine; Japan Yellow 202(1); Obiturine; Resorcinol phthalein sodium; Sodium fluorescein; Sodium fluoresceinate; Soluble Fluorescein; Soluble Fluoresceine BPS; Uranin; Uranin A; Uranin Conc; Uranin S; Uranine; Uranine A; Uranine A extra; Uranine O; Uranine SS; Uranine WSS

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-, disodium salt

**CAS Registry Number** 518-47-8

**Merck Index Number** 4159

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula**  $C_{20}H_{10}O_5Na_2$

**Molecular Weight** 376.28

**pH Range** 4.0–6.0

**Color Change at pH** Pink fluorescence (4.0) to green fluorescence (6.0)

**pKa** 2.2, 4.4, 6.7

**Physical Form** Orange-red powder

**Solubility** Freely soluble in water; slightly soluble in ethanol

**UV-Visible ( $\lambda_{max}$ )** 491 nm, 493.5 nm, 490 nm

**Melting Point** >300°C

**Synthesis** Synthetic methods<sup>1–4</sup>

**Major Applications** Nanolithography,<sup>5</sup> nanoparticles,<sup>6</sup> thin films,<sup>7</sup> fuel cells,<sup>8</sup> inks,<sup>9</sup> laser,<sup>10</sup> colored bubbles,<sup>11</sup> cleansing products,<sup>12</sup> identifying leaks in coolant,<sup>13</sup> suntanning agent,<sup>14</sup> hair dyes,<sup>15</sup> cosmetics,<sup>16</sup> dermatology,<sup>17</sup> dental material,<sup>18</sup> diagnosis of diabetic retinopathy,<sup>19</sup> antitumor agent<sup>20</sup>

**Safety/Toxicity** Acute and chronic toxicity,<sup>21</sup> ecotoxicity,<sup>22</sup> hemorheological effects,<sup>23</sup> toxicity to insects,<sup>24</sup> mutagenicity,<sup>25</sup> carcinogenicity,<sup>25</sup> chromosome aberration,<sup>26</sup> phototoxicity<sup>27</sup>

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## FLUORESC EIN-5-ISOTHIOCYANATE (FITC)

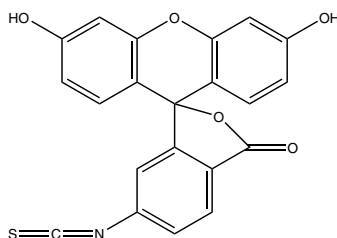
**Other Names** Fluorescein, 5-isothiocyanato-; 5-Isothiocyanatofluorescein; FITC isomer I; Fluorescein 5-isothiocyanate; Fluorescein isothiocyanate isomer 1; Fluorescein isothiocyanate isomer I; Fluorescein-5-isothiocyanate

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-5-isothiocyanato-

**CAS Registry Number** 3326-32-7

**Merck Index Number** 4089

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>21</sub>H<sub>11</sub>NO<sub>5</sub>S

**Molecular Weight** 389.38

**pH Range** 6.0–7.2

**Color Change at pH** Weak green fluorescence (6.0) to strong green fluorescence (7.2)

**pKa** 2.2, 4.4, 6.7

**Physical Form** Orange powder

**Solubility** Insoluble in water; soluble in ethanol, acetone, *N,N*-dimethylformamide

**UV-Visible** ( $\lambda_{\text{max}}$ ) 490 nm

**Melting Point** >360°C

**Boiling Point (Calcd.)** 708.6 ± 60.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Magnetic nanowires,<sup>6</sup> immunoassays,<sup>7</sup> analyzing proteins,<sup>8</sup> identifying chromosomes,<sup>9</sup> diagnosis of cancer,<sup>10</sup> kidney diseases,<sup>11</sup> detecting pathogens,<sup>12</sup> genes,<sup>13</sup> *Salmonella* cells,<sup>14</sup> toxoplasmosis,<sup>15</sup> enzyme-mediated nucleic acid cleavage,<sup>16</sup> surface molecules on colorectal cancers,<sup>17</sup> treating cancer,<sup>18</sup> chronic lymphocytic leukemia<sup>19</sup>

**Safety/Toxicity** Cytotoxicity,<sup>20</sup> genotoxicity,<sup>21</sup> phototoxicity<sup>22</sup>

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## FLUOREXON

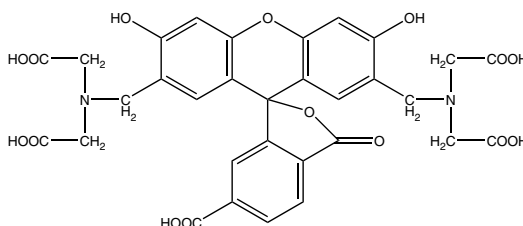
**Other Names** Fluorescein, 2',7'-bis[[bis(carboxymethyl)amino]methyl]-; Spiro[isobenzofuran-1(3H),9'-[9H]xanthene], glycine deriv.; 2,7-Bis[*N,N*-bis(carboxymethyl)aminomethylene]-fluorescein; Acetic acid, [(3',6'-dihydroxy-2',7'-fluorandiyl)bis-(methylenenitrilo)]tetra-; Calcein; Fluorescein complexon; Fluorexon; NSC 298193; Oftasceine

**CA Index Name** Glycine, *N,N'*-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-2',7'-diyl)bis(methylene)]bis[*N*-(carboxymethyl)-

**CAS Registry Number** 1461-15-0

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>30</sub>H<sub>26</sub>N<sub>2</sub>O<sub>13</sub>

**Molecular Weight** 622.53

**pH Range** 6.0–7.2

**Color Change at pH** Weak green fluorescence (6.0) to strong green fluorescence (7.2)

**pKa** 6.67

**Physical Form** Orange powder

**Solubility** Soluble in water, ethanol

**UV-Visible (λ<sub>max</sub>)** 494 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 952.7 ± 65.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–6</sup>

**Major Applications** Chemical–mechanical polishing,<sup>7,8</sup> stabilizing liposomes,<sup>9</sup> cell motility assay,<sup>10</sup> detecting nucleic acids,<sup>11</sup> virus,<sup>12</sup> screening safety of gastric mucosa,<sup>13</sup> MDR inhibitors,<sup>14</sup> drug delivery,<sup>15</sup> imaging atherosclerotic plaque<sup>16</sup>

**Safety/Toxicity** Cytotoxicity,<sup>17</sup> exitotoxicity<sup>18</sup>

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# G

## GALLEIN

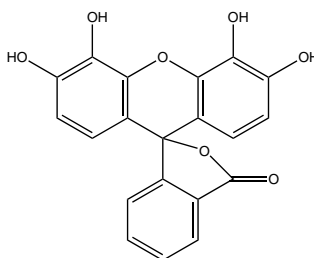
**Other Names** Gallein; Alizarine violet; C.I. 45445; C.I. Mordant Violet 25; Mordant Violet 25; NSC 56445; NSC 622478; NSC 8668; Pyrogallolphthalein

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',4',5',6'-tetrahydroxy-

**CAS Registry Number** 2103-64-2

**Merck Index Number** 4344

### Chemical Structure



**Chemical/Dye Class** Miscellaneous, Xanthene

**Molecular Formula** C<sub>20</sub>H<sub>12</sub>O<sub>7</sub>

**Molecular Weight** 364.31

**pH Range** 3.8–6.6;  
10.6–13.0

**Color Change at pH** Yellow (3.8) to rose-red (6.6)  
Pink (10.6) to violet (13.0)

**pKa** 5.99

**Physical Form** Brownish-red powder

**Solubility** Almost insoluble in water, benzene, chloroform; soluble in ethanol, acetone

**UV-Visible** ( $\lambda_{\text{max}}$ ) 526 nm

**Melting Point** >300°C

**Boiling Point (Calcd.)** 687.4 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–7</sup>

**Major Applications** Organic light emitting devices (OLED),<sup>8</sup> semiconductors,<sup>9,10</sup> photoresists,<sup>11,12</sup> lithographic printing plates,<sup>13</sup> method for ozone determination,<sup>14</sup> treatment of wastewater,<sup>15</sup> determination of silver,<sup>16</sup> nail polish,<sup>17</sup> monitoring sterilization,<sup>18</sup> determination of proteins,<sup>19</sup> induce apoptosis in cancer cells,<sup>20</sup> treatment of cancer cells,<sup>21</sup> antiHIV agent,<sup>22</sup> diagnosis and treatment of amyloidosis,<sup>23</sup> cancer chemo preventive activity,<sup>24</sup> drug design,<sup>25</sup> inhibition of influenza virus<sup>26</sup>

**Safety/Toxicity** No data available

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## GENTIAN VIOLET

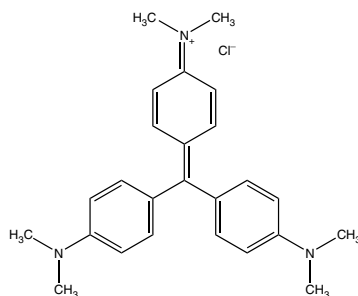
**Other Names** C.I. Basic Violet 3; 12416 Violet; Adergon; Aizen Crystal Violet; Aizen Crystal Violet Extra Pure; Aniline violet; Aniline violet pyoktanine; Atmonil; Avermin; Axuris; Badil; Basic Violet 3; Basic Violet BN; Basonyl Violet 610; C.I. 42555; Calcozine Violet 6BN; Calcozine Violet C; Crystal Violet 10B; Crystal Violet 5BO; Crystal Violet 6B; Crystal Violet 6BO; Crystal Violet AO; Crystal Violet AON; Crystal Violet BP; Crystal Violet BPC; Crystal Violet Extra Pure; Crystal Violet Extra Pure APN; Crystal Violet Extra Pure APNX; Crystal Violet FN; Crystal Violet HL 2; Crystal Violet O; Crystal Violet Pure DSC; Crystal Violet Pure DSC Brilliant; Crystal Violet SS; Crystal Violet Technical; Crystal Violet USP; Crystal Violet chloride; Crystal violet; Gentersal; Gentian Violet B; Gentian violet; Gentiaverm; Gentacid; Gentioletten; Hecto Violet R; Hectograph Violet SR; Hexamethyl violet; Hexamethyl-*p*-rosaniline chloride; Hexamethylpararosaniline chloride; Hidaco Brilliant Crystal Violet; Meroxyl; Meroxyl-Wander; Meroxylan; Meroxylan-Wander; Methyl Violet 10B; Methyl Violet 10BD; Methyl Violet 10BK; Methyl Violet 10BN; Methyl Violet 10BNS; Methyl Violet 10BO; Methyl Violet 5BNO; Methyl Violet 5BO; Methyl Violet 6B; Methyl Violet 6B (biological stain); Methylrosaniline chloride; Methylrosanilinium chloride; Mitsui Crystal Violet; Oxiuran; Oxycolor; Oxyozyl; Paper Blue R; Pararosaniline, N,N,N',N',N'',N''-hexamethyl-, chloride; Plastoresin Violet 5BO; Pyoktanin; Sanyo Fanal Violet R; Vermicid; Vianin; Viocid; Violet 5BO; Violet 6BN; Violet CP; Violet XXIII; crystal violet

**CA Index Name** Methanaminium, N-[4-[bis[4-(dimethylamino)phenyl]methylene]-2,5-cyclohexadien-1-ylidene]-N-methyl-, chloride

**CAS Registry Number** 548-62-9

**Merck Index Number** 4395

### Chemical Structure



**Chemical/Dye Class** Triphenylmethane

**Molecular Formula** C<sub>25</sub>H<sub>30</sub>N<sub>3</sub>Cl

**Molecular Weight** 407.99

**pH Range** 0.0–2.0

**Color Change at pH** Yellow (0.0) to blue-violet (2.0)

**pKa** 9.4

**Physical Form** Green to yellowish-green powder

**Solubility** Soluble in water, acetone, chloroform; very soluble in ethanol; practically insoluble in ether; insoluble in xylene

**UV-Visible (λ<sub>max</sub>)** 590 nm

**Melting Point** 205–215°C (decompose)

**Synthesis** Synthetic methods<sup>1–12</sup>

**Major Applications** Photoresists,<sup>13</sup> lithographic printing plate,<sup>14</sup> printed circuit board,<sup>15</sup> inks,<sup>16</sup> detergent,<sup>17</sup> hair dyes,<sup>18</sup> shampoo,<sup>19</sup> drug screening method,<sup>20</sup> bone cement preparation method,<sup>21</sup> treating microorganisms,<sup>22</sup> hemorrhoids,<sup>23</sup> antifungal,<sup>24</sup> antibacterial,<sup>25</sup> antimalarial agent,<sup>26</sup> dental application<sup>27</sup>

**Safety/Toxicity** Acute oral toxicity,<sup>28</sup> chronic toxicity,<sup>29,30</sup> carcinogenicity,<sup>29,30</sup> cytotoxicity,<sup>31</sup> genotoxicity,<sup>32</sup> mutagenicity,<sup>33,34</sup> ototoxicity,<sup>35</sup> percutaneous toxicity,<sup>36</sup> phototoxicity<sup>37</sup>

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## GENTIAN VIOLET B

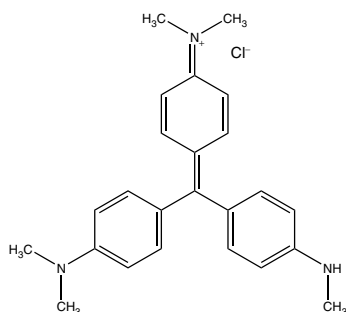
**Other Names** Methyl violet; Aizen Methyl Violet BB; Aizen Methyl Violet Pure Special; Basic Violet 1; Basic Violet 5BN; Basic Violet K; Basonyl Violet 600; C Ext. Violet 5; C.I. 42535; Gentian Violet B; Methyl Violet 2B; Methyl Violet 6B; Methyl Violet B; Methyl Violet BB; Methyl Violet FN; Methyl Violet N; Methyl Violet Pure Special; Methyl Violet pure SP; Paris Violet R; Pyoktanin blue; Pyoktaninum coeruleum; Violet Powder H 2503

**CA Index Name** C.I. Basic Violet 1

**CAS Registry Number** 8004-87-3

**Merck Index Number** Not listed

**Chemical Structure** It is a mixture of *N*-pentamethyl (as shown) and *N*-hexamethyl (which is Crystal Violet) *p*-rosaniline chlorides



**Chemical/Dye Class** Triphenylmethane

**Molecular Formula** Mixture of tetra-, penta-, and hexamethyl *p*-rosaniline chlorides

**Molecular Weight** Mixture of tetra-, penta-, and hexamethyl *p*-rosaniline chlorides

**pH Range** 0.15–3.2

**Color Change at pH** Yellow (0.15) to violet (3.2)

**Physical Form** Green crystals

**Solubility** Soluble in water, ethanol, chloroform; insoluble in ether, xylene

**UV-Visible** ( $\lambda_{\text{max}}$ ) 584 nm

**Melting Point** 137°C (decompose)

**Synthesis** Synthetic methods<sup>1–6</sup>

**Major Applications** Display device,<sup>7,8</sup> photoresists,<sup>9</sup> solar cells,<sup>10</sup> inks,<sup>11,12</sup> highlighters,<sup>13</sup> rubber,<sup>14</sup> lithium battery,<sup>15</sup> petroleum products,<sup>16</sup> leak detection method,<sup>17</sup> decoder system,<sup>18</sup> packaging materials,<sup>19</sup> hair dyes,<sup>20</sup> cosmetics,<sup>21</sup> wound dressing materials,<sup>22</sup> antitumor agent,<sup>23</sup> determination of nucleic acids<sup>24</sup>

**Safety/Toxicity** Acute toxicity,<sup>25</sup> carcinogenicity,<sup>26</sup> toxicity to aquatic microbes,<sup>27</sup> mutagenicity<sup>28</sup>

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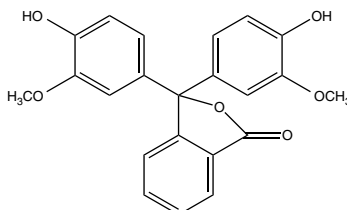
## GUAIACOLPHTHALEIN

**Other Names** Phenolphthalein, 3',3''-dimethoxy-; 3',3''-Dimethoxyphenolphthalein; Guaiacolphthalein

**CA Index Name** 1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxy-3-methoxyphenyl)-

**CAS Registry Number** 467-25-4

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Phthalein

**Molecular Formula** C<sub>22</sub>H<sub>18</sub>O<sub>6</sub>

**Molecular Weight** 378.37

**pH Range** 8.4–10.2

**Color Change at pH** Colorless (8.4) to violet-blue (10.2)

**pKa** 9.7

**Physical Form** White powder

**Solubility** Insoluble in water; soluble in ethanol, methanol

**Melting Point** >300°C

**Boiling Point (Calcd.)** 602.2 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic method<sup>1,2</sup>

**Major Applications** Toner,<sup>3</sup> toothpaste & mouthwash,<sup>4</sup> disinfectant,<sup>5</sup> cosmetics,<sup>6</sup> paints<sup>7</sup>

**Safety/Toxicity** No data available

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# H

## HARMINE

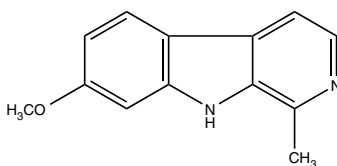
**Other Names** 1-Methyl-7-methoxy- $\beta$ -carboline; 7-Methoxy-1-methyl-9H-pyrido[3,4-b]indole; Banisterin; Banisterine; Harmin; Harmine; Leucoharmine; Telepathin; Telepathine; Yagein; Yageine

**CA Index Name** 9H-Pyrido[3,4-b]indole, 7-methoxy-1-methyl-

**CAS Registry Number** 442-51-3

**Merck Index Number** 4616

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Heterocyclic

**Molecular Formula** C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O

**Molecular Weight** 212.25

**pH Range** 7.2–8.9

**Color Change at pH** Blue fluorescence (7.2) to yellow fluorescence (8.9)

**pKa** 7.7

**Physical Form** White to off-white crystals

**Solubility** Slightly soluble in water, ethanol, ether, chloroform

**UV-Visible** ( $\lambda_{\text{max}}$ ) 241 nm, 301 nm, 336 nm

**Melting Point** 261°C (decompose)

**Boiling Point (Calcd.)** 421.4  $\pm$  40.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–11</sup>

**Major Applications** Inks,<sup>12</sup> antitumor agents,<sup>1,3,7,8,13–15</sup> inhibition of cell proliferation,<sup>16</sup> blocking breast and prostate cancer cells,<sup>17</sup> tracer for ductal pancreatic cancer,<sup>18</sup> DNA binding properties,<sup>19</sup> treatment of neoplasia,<sup>20</sup> antioxidants,<sup>21</sup> therapy of depression,<sup>22</sup> antileishmanial agent,<sup>23,24</sup> treatment of parkinsonism,<sup>25,26</sup> antiAIDS agents,<sup>3,27</sup> antihypoxia agents,<sup>28</sup> drugs,<sup>29</sup> treatment of dependency disorder,<sup>30</sup> psychiatric and neurological illness,<sup>31</sup> antibiotics,<sup>32</sup> antimalarial agents.<sup>33</sup>

**Safety/Toxicity** Neurotoxicity,<sup>7,34,35</sup> nephrotoxicity,<sup>35</sup> cytotoxicity,<sup>36</sup> genotoxicity,<sup>37–39</sup> hepatocarcinogenicity,<sup>40</sup> mutagenicity,<sup>41</sup> hepatotoxicity.<sup>42</sup>

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## HEMATOXYLIN

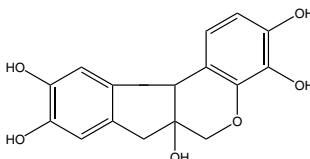
**Other Names** Benz[b]indeno[1,2-d]pyran-3,4,6a,9,10(6H)-pentol, 7,11b-dihydro; Benz[b]indeno[1,2-d]pyran-3,4,6a,9,10(6H)-pentol, 7,11b-dihydro, (6aS-cis)-; (+)-Hematoxylin; Haematoxylin; Hematoxylin; Hematoxyline; Hydroxybrazilin; Hydroxybrazilin; NSC 270085

**CA Index Name** Benz[b]indeno[1,2-d]pyran-3,4,6a,9,10(6H)-pentol, 7,11b-dihydro, (6aS,11bR)-

**CAS Registry Number** 517-28-2

**Merck Index Number** 4637

### Chemical Structure



**Chemical/Dye Class** Miscellaneous, Polymethine, Flavone

**Molecular Formula** C<sub>16</sub>H<sub>14</sub>O<sub>6</sub>

**Molecular Weight** 302.28

**pH Range** 0.0–1.0;

5.0–6.0

**Color Change at pH** Red (0.0) to yellow (1.0)

Pale yellow (5.0) to violet (6.0)

**pKa** 6.7

**Physical Form** Tan powder

**Solubility** Soluble in water, ethanol, ethylene glycol, methyl cellosolve

**UV-Visible** ( $\lambda_{\text{max}}$ ) 292 nm, 445 nm, 560 nm

**Melting Point** 200°C (decompose)

**Boiling Point (Calcd.)** 579.9 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–6</sup>

**Major Applications** Plasma displays,<sup>7</sup> textiles,<sup>8</sup> hair dyes,<sup>9</sup> identifying fresh and stale rice,<sup>10</sup> diagnosing cancer progression,<sup>11</sup> cervical disease,<sup>12</sup> central nervous system malfunctions,<sup>13</sup> detecting genes,<sup>14</sup> breast cancer,<sup>15</sup> collagen in a tissue sample,<sup>16</sup> apoptosis,<sup>17</sup> demyelinating diseases,<sup>18</sup> antigens,<sup>19</sup> treatment of age-related macular degeneration,<sup>20</sup> burns,<sup>21</sup> prostate cancer,<sup>22</sup> diabetes and obesity,<sup>23</sup> viral diseases,<sup>24</sup> neoplasms,<sup>25</sup> peripheral neural and vascular ailments,<sup>26</sup> skin disorders,<sup>27</sup> biotechnological applications,<sup>28</sup> reference standard materials for cytology, histology and immunohistochemistry<sup>29</sup>

**Safety/Toxicity** Carcinogenicity,<sup>30</sup> genotoxicity,<sup>31</sup> mutagenicity,<sup>32</sup> neurotoxicity<sup>33</sup>

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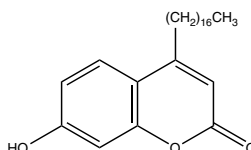
**4-HEPTADECYL-7-HYDROXYCOUMARIN**

**Other Names** Coumarin, 4-heptadecyl-7-hydroxy-; 4-Heptadecyl-7-hydroxycoumarin; 4-Heptadecylumbelliferone

**CA Index Name** 2H-1-Benzopyran-2-one, 4-heptadecyl-7-hydroxy-

**CAS Registry Number** 26038-83-5

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Fluorescent, Coumarin

**Molecular Formula** C<sub>26</sub>H<sub>40</sub>O<sub>3</sub>

**Molecular Weight** 400.59

**pH Range** 7.9–9.9

**Color Change at pH** Weak blue fluorescence (7.9) to strong blue fluorescence (9.9)

**pKa** 8.9

**Physical Form** Off-white solid

**Solubility** Insoluble in water; soluble in ethanol, N,N-dimethylformamide, dimethyl sulfoxide

**UV-Visible** ( $\lambda_{\text{max}}$ ) 325 nm, 366 nm

**Melting Point** 95°C

**Boiling Point (Calcd.)** 544.7 ± 45.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Fluorescent probes,<sup>3,4</sup> monolayer assemblies,<sup>5</sup> lipoplex electrostatics,<sup>6</sup> opto-acoustic contrast agents<sup>7</sup>

**Safety/Toxicity** No data available

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## HEPTAMETHOXY RED

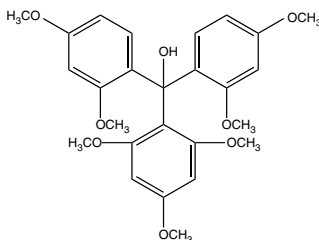
**Other Names** Carbinol, *bis*(2,4-dimethoxyphenyl)(2,4,6-trimethoxyphenyl)-; Heptamethoxy red

**CA Index Name** Benzenemethanol,  $\alpha,\alpha$ -*bis*(2,4-dimethoxyphenyl)-2,4,6-trimethoxy-

**CAS Registry Number** 80202-76-2

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Triphenylmethane

**Molecular Formula** C<sub>26</sub>H<sub>30</sub>O<sub>8</sub>

**Molecular Weight** 470.51

**pH Range** 5.0–7.0

**Color Change at pH** Red (5.0) to colorless (7.0)

**pKa** 5.9

**Physical Form** White crystalline powder

**Solubility** Insoluble in water; soluble in ethanol

**Melting Point** 149°C

**Boiling Point (Calcd.)** 652.2 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Recording materials,<sup>3</sup> inks<sup>4,5</sup>

**Safety/Toxicity** No data available

### References

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5. Kawashima, S. Printing inks with changing colors. Jpn. Kokai Tokkyo Koho JP 02266389, 1990; *Chem. Abstr.* **1991**, *114*, 145649.

## HEXAMETHOXY RED

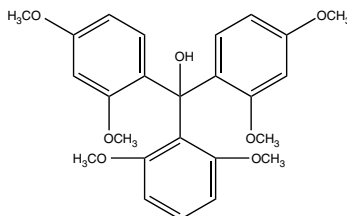
**Other Names** Hexamethoxytriphenylcarbinol

**CA Index Name** Benzenemethanol,  $\alpha,\alpha$ -bis(2,4-dimethoxyphenyl)-2,6-dimethoxy-

**CAS Registry Number** 50814-92-1

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Triphenylmethane

**Molecular Formula** C<sub>25</sub>H<sub>28</sub>O<sub>7</sub>

**Molecular Weight** 440.44

**pH Range** 2.6–4.6

**Color Change at pH** Reddish-pink (2.6) to colorless (4.6)

**pKa** 3.3

**Physical Form** White crystalline powder

**Solubility** Insoluble in water, soluble in ethanol

**Melting Point** 147°C

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Inks<sup>2–4</sup>

**Safety/Toxicity** No data available

## References

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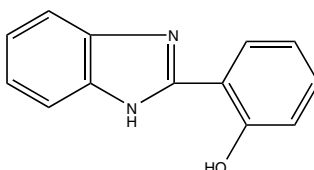
**o-HYDROXYPHENYLBENZIMIDAZOLE**

**Other Names** Phenol, o-2-benzimidazolyl-; 2-(1H-Benzimidazol-2-yl)phenol; 2-(2'-Hydroxyphenyl)benzimidazole; 2-(2-Benzimidazolyl)phenol; 2-(2-Hydroxyphenyl)-1H-benzimidazole; 2-(2-Hydroxyphenyl)-benzimidazole; 2-(o-Hydroxyphenyl)-benzimidazole; HBI; NSC 32819

**CA Index Name** Phenol, 2-(1H-benzimidazol-2-yl)-

**CAS Registry Number** 2963-66-8

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>13</sub>H<sub>10</sub>N<sub>2</sub>O

**Molecular Weight** 210.23

**pH Range** -9.9-

**Color Change at pH** Nonfluorescence (<9.9) to blue-violet fluorescence (9.9)

**pKa** 9.23

**Physical Form** White to tan crystals

**Solubility** Insoluble in water; soluble in ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 245 nm, 300 nm

**Melting Point** 240–242°C

**Boiling Point (Calcd.)** 444.2 ± 47.0°C Pressure: 760

**Synthesis** Synthetic methods<sup>1-6</sup>

**Major Applications** Optical devices,<sup>7</sup> photography,<sup>8</sup> plastic scintillation applications,<sup>9</sup> fungicide,<sup>10</sup> antiviral agent,<sup>11</sup> antiinflammatory agent,<sup>12</sup> antibacterial agent<sup>12</sup>

**Safety/Toxicity** Acute toxicity<sup>13</sup>

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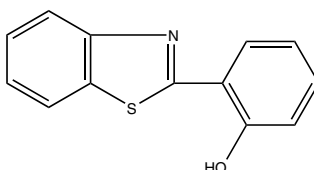
**o-HYDROXYPHENYLBENZOTHAZOLE**

**OtherNames** Phenol, o-2-benzothiazolyl-; 2-(2'-Hydroxyphenyl)benzothiazole; 2-(2-Benzothiazolyl)phenol; 2-(2-Hydroxyphenyl)benzothiazole; 2-(o-Hydroxyphenyl)benzothiazole; HBT; NSC 5051; NSC 58548

**CA Index Name** Phenol, 2-(2-benzothiazolyl)-

**CAS Registry Number** 3411-95-8

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>13</sub>H<sub>9</sub>NOS

**Molecular Weight** 227.28

**pH Range** -9.3-

**Color Change at pH** Nonfluorescence (<9.3) to blue-green fluorescence (9.3)

**pKa** 8.21

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in ethanol

**Melting Point** 130–132°C

**Boiling Point (Calcd.)** 402.2 ± 47.0°C Pressure: 760

**Synthesis** Synthetic methods<sup>1–6</sup>

**Major Applications** Organic light emitting devices,<sup>7,8</sup> electroluminescent devices,<sup>9,10</sup> laser dyes,<sup>11</sup> photography,<sup>12</sup> plastic scintillation applications,<sup>13</sup> herbicides,<sup>14</sup> eyeglass lenses,<sup>15</sup> cosmetics<sup>16</sup>

**Safety/Toxicity** Endocrine disrupters<sup>17</sup>

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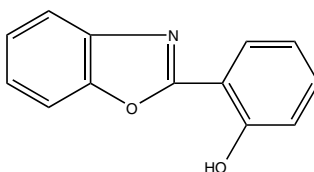
**o-HYDROXYPHENYLBENZOXAZOLE**

**Other Names** Phenol, *o*-2-benzoxazolyl-; 2-(1,3-Benzoxazol-2-yl)phenol; 2-(2'-Hydroxyphenyl)benzoxazole; 2-(2-Hydroxyphenyl)benzoxazole; 2-(*o*-Hydroxyphenyl)benzoxazole; HBO; NSC 403545; NSC 5423; *o*-2-Benzoxazolylphenol

**CA Index Name** Phenol, 2-(2-benzoxazolyl)-

**CAS Registry Number** 835-64-3

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>13</sub>H<sub>9</sub>NO<sub>2</sub>

**Molecular Weight** 211.22

**pH Range** -9.3-

**Color Change at pH** Nonfluorescence (<9.3) to blue-violet fluorescence (9.3)

**pKa** 8.04

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in ethanol

**Melting Point** 125–126°C

**Boiling Point** 338°C

**Synthesis** Synthetic methods<sup>1–8</sup>

**Major Applications** Electroluminescent devices,<sup>9,10</sup> reflective films,<sup>11</sup> sensors,<sup>12</sup> plastic scintillation applications,<sup>13</sup> antitumor agent,<sup>14</sup> antibacterial agent<sup>14</sup>

**Safety/Toxicity** No data available

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## INDIGO CARMINE

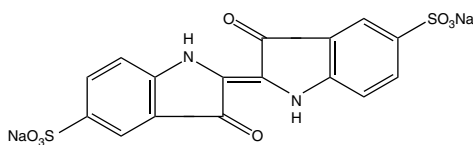
**Other Names** C.I. Acid Blue 74; [ $\Delta$ 2,2'-Biindoline]-5,5'-disulfonic acid, 3,3'-dioxo-, disodium salt; 12070 Blue; 1311 Blue; 5,5'-Indigodisulfonic acid disodium salt; A.F. Blue No. 2; Acid Blue 74; Acid Blue W; Acid Leather Blue IC; Airedale Blue IN; Amacid Brilliant Blue; Aniline Carmine Powder; Ariavit Indigo Carmine; Atul Indigo Carmine; Bucacid Indigotine B; C.I. 73015; C.I. 75781; C.I. Food Blue 1; C.I. Natural Blue 2; Canacert Indigo Carmine; Carmine Blue; Cilefa Blue R; Disodium 5,5'-indigodisulfonate; Disodium 5,5'-indigotin disulfonate; Dolkwal Indigo Carmine; E 132; Edicol Supra Blue X; FD & C Blue 2; FD and C Blue 2; FD and C Blue No. 2; FD&C Blue No. 2; Food Blue 1; Food Blue 2; Food Blue No. 1; Food Blue No. 2; Grape Blue A; HD Indigo Carmine; HD Indigo Carmine Supra; Hexacert Blue No. 2; Hexacol Indigo Carmine Supra; Indigo Carmine A; Indigo Carmine AC; Indigo Carmine BP; Indigo Carmine Conc. FQ; Indigo Carmine Powder; Indigo Carmine X; Indigo Extract; Indigo carmine; Indigo carmine NB; Indigotin; Indigotin (solubilized); Indigotine; Indigotine B; Indigotine Blue LZ; Indigotine Carmine; Indigotine Extra Pure A; Indigotine I; Indigotine IA; Indigotine Lake; Indigotine N; Indigotine disodium salt; Indocarmine F; Intense Blue; Japan Blue 2; L Blue Z 5010; Maple Indigo Carmine; Mitsui Indigo Carmine; San-ei Indigo Carmine; Sodium 5,5'-indigodisulfonate; Sodium 5,5'-indigotindisulfonate; Soluble indigo; Soluble indigo blue; Sumitomo Wool Blue SBC; Usacert Blue No. 2; Usacert FD and C Blue No. 2; WAS 35

**CA Index Name** 1H-Indole-5-sulfonic acid, 2-(1,3-dihydro-3-oxo-5-sulfo-2H-indol-2-ylidene)-2,3-dihydro-3-oxo-, disodium salt

**CAS Registry Number** 860-22-0

**Merck Index Number** 4944

**Chemical Structure**



**Chemical/Dye Class** Miscellaneous, Indigoid

**Molecular Formula**  $C_{16}H_8N_2O_8S_2Na_2$

**Molecular Weight** 466.36

**pH Range** 11.5–14.0

**Color Change at pH** Blue (11.5) to yellow (14.0)

**Physical Form** Blue-purple powder

**Solubility** Soluble in water, ethanol

**UV-Visible ( $\lambda_{max}$ )** 608 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1-9</sup>

**Major Applications** Display device,<sup>10</sup> sensor,<sup>11</sup> chemical-mechanical polishing,<sup>12</sup> batteries,<sup>13</sup> photographic materials,<sup>14</sup> thermoplastics,<sup>15</sup> inks,<sup>16</sup> highlighters,<sup>17</sup> detergents,<sup>18</sup> disinfectants,<sup>19</sup> rodenticide,<sup>20</sup> colored bubbles,<sup>21</sup> hair dyes,<sup>22</sup> cosmetics,<sup>23</sup> food,<sup>24</sup> determine bacterial growth,<sup>25</sup> antiischemic agents,<sup>26</sup> antiseptic,<sup>27</sup> antitumor agents,<sup>28</sup> Alzheimer's disease,<sup>29</sup> psychoactive drugs,<sup>30</sup> Tooth whitening,<sup>31</sup> oral care agent<sup>32</sup>

**Safety/Toxicity** Toxicity to reproductive system,<sup>33</sup> carcinogenicity,<sup>34</sup> cytotoxicity,<sup>35</sup> genotoxicity,<sup>36</sup> hypotension,<sup>37</sup> hypertension,<sup>38</sup> mutagenicity,<sup>39</sup> teratogenicity<sup>40</sup>

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## INDOPHENOL

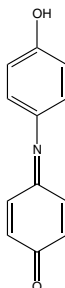
**Other Names** Indophenol; Benzenoneindophenol; Phenolindophenol

**CA Index Name** 2,5-Cyclohexadien-1-one, 4-[(4-hydroxyphenyl)imino]-

**CAS Registry Number** 500-85-6

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Miscellaneous

**Molecular Formula** C<sub>12</sub>H<sub>9</sub>NO<sub>2</sub>

**Molecular Weight** 199.21

**pH Range** 6.3–12.3

**Color Change at pH** Red (6.3) to blue (12.3)

**pKa** 8.1, 9.4, 10.6

**Physical Form** Reddish-blue powder

**Solubility** Insoluble in water; soluble in ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 602 nm

**Melting Point** >300°C

**Boiling Point (Calcd.)** 360.0 ± 42.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1-3</sup>

**Major Applications** Liquid crystal display device,<sup>4</sup> chemical-mechanical polishing,<sup>5</sup> fuel cell,<sup>6</sup> redox materials,<sup>7</sup> hair dyes,<sup>8</sup> lubricants,<sup>9</sup> bacterial vaginosis screening technique,<sup>10</sup> biosensor<sup>11</sup>

**Safety/Toxicity** Environmental pollutants,<sup>12</sup> toxicity to fish<sup>13</sup>

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## IODOPHENOL BLUE

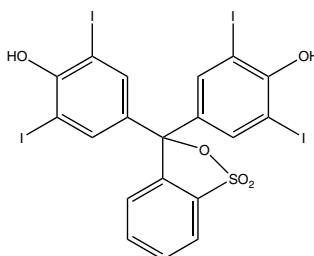
**Other Names** Iodophenol blue; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2,6-diiodo-, S,S-dioxide; 3H-2,1-Benzoxathiole, phenol deriv.; NSC 36792, Tetraiodophenolsulfonephthalein

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2,6-diiodo-

**CAS Registry Number** 4430-24-4

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula**  $C_{19}H_{10}I_4O_5S$

**Molecular Weight** 857.96

**pH Range** 3.0–4.8

**Color Change at pH** yellow (3.0) to blue (4.8)

**pKa** 4.16

**Physical Form** Brown powder

**Solubility** Slightly soluble in water; soluble in ethanol, methanol, acetone, ether, acetic acid

**UV-Visible ( $\lambda_{max}$ )** 433 nm

**Melting Point** 229°C (decompose)

**Boiling Point (Calcd.)**  $615.3 \pm 55.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Shelf life indicator,<sup>2</sup> determining proteins,<sup>3</sup> human serum albumins,<sup>4</sup> polymeric biguanides,<sup>5</sup> examining renal and hepatic functions,<sup>6</sup> apoptosis assay<sup>7</sup>

**Safety/Toxicity** No data available

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## ISONITROSOTHIOCAMPHOR

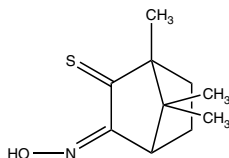
**Other Names** 2,3-Bornanedione, 2-thio-, 3-oxime; Isonitrosothiocamphor

**CA Index Name** Bicyclo[2.2.1]heptan-2-one, 4,7,7-trimethyl-3-thioxo-, oxime

**CAS Registry Number** 91156-63-7

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Miscellaneous

**Molecular Formula**  $C_{10}H_{15}NOS$

**Molecular Weight** 197.30

**pH Range** 8.6–9.0

**Color Change at pH** Violet (8.6) to yellow (9.0)

**pKa** 9.42

**Physical Form** Violet crystals

**Solubility** Soluble in water, ethanol

**Melting Point** 148°C

**Boiling Point (Calcd.)**  $292.1 \pm 23.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Reagent for rhodium,<sup>2</sup> platinum,<sup>3</sup> cobalt,<sup>4</sup> palladium,<sup>5</sup> copper,<sup>6</sup> cadmium,<sup>7</sup> nickel<sup>8</sup>

**Safety/Toxicity** No data available

### References

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## ISOPICRAMIC ACID

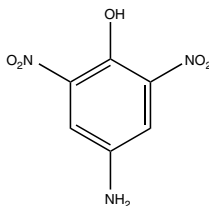
**Other Names** 4-Amino-2,6-dinitrophenol; Isopicramic acid

**CA Index Name** Phenol, 4-amino-2,6-dinitro-

**CAS Registry Number** 17973-92-1

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Nitro

**Molecular Formula**  $C_6H_5N_3O_5$

**Molecular Weight** 199.12

**pH Range** 4.0–5.6

**Color Change at pH** Rose-pink (4.0) to yellow (5.6)

**pKa** 5.09

**Physical Form** Orange-brown powder

**Solubility** Insoluble in water; soluble in ethanol

**Melting Point**  $>250^{\circ}\text{C}$

**Boiling Point (Calcd.)**  $356.9 \pm 42.0^{\circ}\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Toys<sup>3</sup>

**Safety/Toxicity** No data available

## References

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# L

## LACMOID

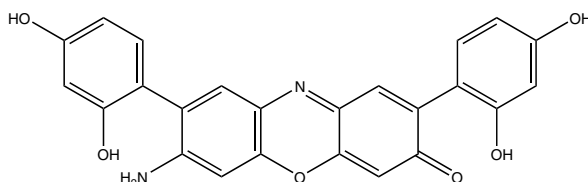
**Other Names** 2-Amino-3,6-bis(2,4-dihydroxyphenyl)-2-phenoxazone; Fluorescent Blue; Iris Blue B; Lacmoid; Resorcein; Resorcein Blue

**CA Index Name** 3H-Phenoxazin-3-one, 7-amino-2,8-bis(2,4-dihydroxyphenyl)-

**CAS Registry Number** 33869-21-5

**Merck Index Number** 5332

### Chemical Structure



**Chemical/Dye Class** Miscellaneous

**Molecular Formula**  $C_{24}H_{16}N_2O_6$

**Molecular Weight** 428.39

**pH Range** 4.4–6.4

**Color Change at pH** Red (4.4) to blue (6.4)

**pKa** 5.31

**Physical Form** Black-violet powder

**Solubility** Sparingly soluble in water, ether; soluble in water, ethanol, methanol, amyl alcohol, acetone, acetic acid; practically insoluble in chloroform, benzene, petroleum ether

**UV-Visible ( $\lambda_{\max}$ )** 611 nm

**Melting Point**  $>250^\circ\text{C}$

**Boiling Point (Calcd.)**  $755.3 \pm 60.0^\circ\text{C}$  Pressure: 760

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Electrochromic devices,<sup>4</sup> photosensitive materials,<sup>5</sup> parasiticides,<sup>6</sup> hair dyes,<sup>7</sup> cosmetics,<sup>8</sup> ointment for hemorrhoids<sup>9</sup>

**Safety/Toxicity** Fish toxicity<sup>10</sup>

### References

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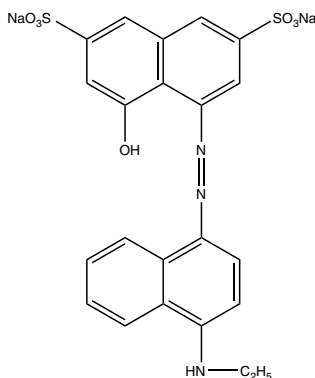
**LANACYL VIOLET BF**

**Other Names** 2,7-Naphthalenedisulfonic acid, 4-[[4-(ethylamino)-1-naphthyl]-azo]-5-hydroxy-, disodium salt; C.I. 13375; Lanacyl Violet BF

**CA Index Name** 2,7-Naphthalenedisulfonic acid, 4-[[4-(ethylamino)-1-naphthalenyl]azo]-5-hydroxy-, disodium salt

**CAS Registry Number** 10214-18-3

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>22</sub>H<sub>17</sub>N<sub>3</sub>O<sub>7</sub>S<sub>2</sub>Na<sub>2</sub>

**Molecular Weight** 545.49

**pH Range** 11.0–13.0

**Color Change at pH** Violet (11.0) to orange (13.0)

**pKa** 12.12

**Physical Form** Solid

**Solubility** Soluble in water, ethanol

**Melting Point** >250°C

**Synthesis** No data available

**Major Applications** No data available

**Safety/Toxicity** No data available

**Reference**

No reference available

## LUMINOL

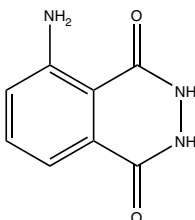
**Other Names** 3-Aminophthalhydrazide; 3-Aminophthalic acid hydrazide; 3-Aminophthalic hydrazide; 5-Amino-1,4-dihydroxyphthalazine; 5-Amino-2,3-dihydro-1,4-phthalazinedione; Luminol; NSC 5064

**CA Index Name** 1,4-Phthalazinedione, 5-amino-2,3-dihydro-

**CAS Registry Number** 521-31-3

**Merck Index Number** 5600

**Chemical Structure**



**Chemical/Dye Class** Fluorescent

**Molecular Formula**  $C_8H_7N_3O_2$

**Molecular Weight** 177.16

**pH Range** 6.0–7.0

**Color Change at pH** Nonfluorescence (6.0) to blue fluorescence (7.0)

**pKa (Calcd.)**  $10.50 \pm 0.20$ ;

$0.58 \pm 0.20$

**Physical Form** Off-white to yellow powder

**Solubility** Insoluble in water, soluble in dimethyl sulfoxide, base

**UV-Visible ( $\lambda_{\max}$ )** 425 nm

**Melting Point** 319–320°C

**Synthesis** Synthetic methods<sup>1–12</sup>

**Major Applications** Night vision devices,<sup>13</sup> identification of product forgeries,<sup>14</sup> determination of nitride in food,<sup>15</sup> analytical chemistry,<sup>16</sup> pharmaceuticals,<sup>17</sup> iodine in biological materials,<sup>18</sup> evaluating phagocytes,<sup>19</sup> detecting tumors,<sup>20</sup> DNA,<sup>21</sup> biosensors,<sup>22,23</sup> assay of fungi,<sup>24</sup> bacteria,<sup>24</sup> yeasts,<sup>24</sup> assay of lipase activity<sup>25</sup>

**Safety/Toxicity** *In vitro* biological effects,<sup>26</sup> cytotoxicity,<sup>27</sup> pulmonary toxicity,<sup>28</sup> mutagenicity,<sup>29,30</sup> neurotoxicity<sup>31</sup>

## References

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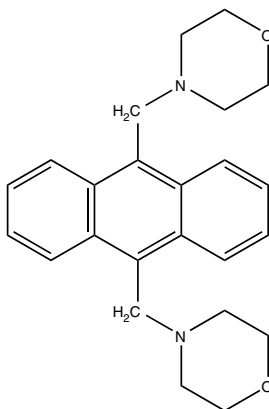
**LYSOSENSOR BLUE DND 167**

**Other Names** Morpholine, 4,4'-(9,10-anthrylenedimethylene)di-; LysoSensor Blue DND 167

**CA Index Name** Morpholine, 4,4'-[9,10-anthracenediylbis(methylene)]bis-

**CAS Registry Number** 101821-61-8

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>24</sub>H<sub>28</sub>N<sub>2</sub>O<sub>2</sub>

**Molecular Weight** 376.49

**pH Range** 4.5–6.0

**Color Change at pH** Strong blue fluorescence (4.5) to weak blue fluorescence (6.0)

**pKa** 5.1

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in dimethyl sulfoxide

**UV-Visible** ( $\lambda_{\text{max}}$ ) 373 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 546.5 ± 45.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Multifunctional reference system,<sup>4</sup> pH probes for acidic organelles in living cells,<sup>5</sup> methods for measuring & controlling multidrug resistance (MDR) of tumor cells,<sup>6,7</sup> fluorescence lifetime characterization of lysosomal pH<sup>8</sup>

**Safety/Toxicity** No data available

**References**

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**LYSOSENSOR BLUE DND 192**

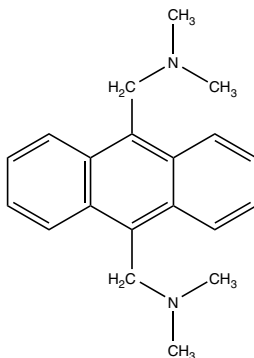
**Other Names** LysoSensor DND 192

**CA Index Name** 9,10-Anthracenedimethanamine, *N,N,N',N'*-tetramethyl-

**CAS Registry Number** 166821-89-2

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>20</sub>H<sub>24</sub>N<sub>2</sub>

**Molecular Weight** 292.42

**pH Range** 6.5–8.5

**Color Change at pH** Strong blue fluorescence (6.5) to weak blue fluorescence (8.5)

**pKa** 7.5

**Physical Form** Solid

**Solubility** Insoluble in water; Soluble in dimethyl sulfoxide

**UV-Visible** ( $\lambda_{\text{max}}$ ) 374 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 418.0 ± 25.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Fluorescence lifetime characterization of lysosomal pH<sup>3</sup>

**Safety/Toxicity** No data available

**References**

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**LYSOSENSOR GREEN DND 189**

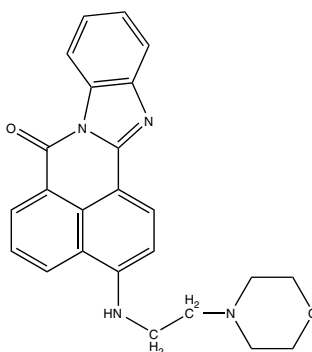
**Other Names** LysoSensor Green DND 189

**CA Index Name** 7H-Benzimidazo[2,1-a]benz[de]isoquinolin-7-one, 3-[[2-(4-morpholinyl)ethyl]amino]-

**CAS Registry Number** 152584-38-8

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>24</sub>H<sub>22</sub>N<sub>4</sub>O<sub>2</sub>

**Molecular Weight** 398.46

**pH Range** 4.5–6.0

**Color Change at pH** Strong green fluorescence (4.5) to weak green fluorescence (6.0)

**pKa** 5.2

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in dimethyl sulfoxide

**UV-Visible ( $\lambda_{\text{max}}$ )** 443 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 704.9 ± 70.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1</sup>

**Major Applications** Biosensors,<sup>2</sup> pH probes for acidic organelles in living cells,<sup>3</sup> method for quantifying nucleic acid incorporated into target organelle,<sup>4</sup> fluorescence lifetime characterization of lysosomal pH<sup>5</sup>

**Safety/Toxicity** No data available

**References**

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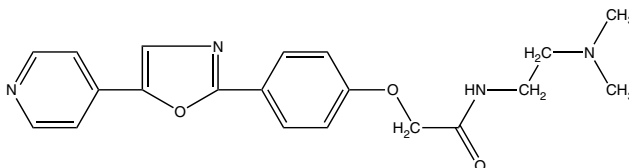
**LYSOSENSOR YELLOW/BLUE DND 160**

**Other Names** L 7545; Lyso Sensor DND 160; LysoSensor Yellow/Blue DND 160; PDMPO

**CA Index Name** Acetamide, *N*-[2-(dimethylamino)ethyl]-2-[4-[5-(4-pyridinyl)-2-oxazolyl]phenoxy]-

**CAS Registry Number** 231632-18-1

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>20</sub>H<sub>22</sub>N<sub>4</sub>O<sub>3</sub>

**Molecular Weight** 366.41

**pH Range** 3.5–6.0

**Color Change at pH** Strong yellow-blue fluorescence (3.5) to weak yellow-blue fluorescence (6.0)

**pKa** 4.2

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in dimethyl sulfoxide

**UV-Visible** ( $\lambda_{\text{max}}$ ) 384 nm, 329 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Recording materials,<sup>3</sup> biosensors,<sup>4</sup> regulating acidity in gastric cells,<sup>5</sup> for biological silicification studies,<sup>1</sup> fluorescence lifetime characterization of lysosomal pH<sup>2</sup>

**Safety/Toxicity** No data available

**References**

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# M

## MAGDALA RED

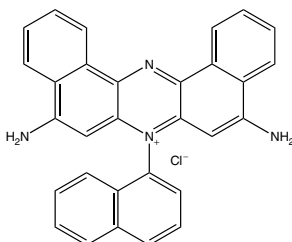
**Other Names** Dibenzo[a,j]phenazinium, 5,9-diamino-7-(1-naphthyl)-, chloride; Magdala Red; Magdaline red; Magdalskaya red

**CA Index Name** Dibenzo[a,j]phenazinium, 5,9-diamino-7-(1-naphthalenyl)-, chloride

**CAS Registry Number** 10114-42-8

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Fluorescent

**Molecular Formula**  $C_{30}H_{21}N_4Cl$

**Molecular Weight** 472.96

**pH Range** 3.0–4.0

**Color Change at pH** Nonfluorescence (3.0) to purple fluorescence (4.0)

**Physical Form** Dark brown powder or green needles

**Solubility** Sparingly soluble in hot water; soluble in ethanol

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1</sup>

**Major Applications** Display device,<sup>2</sup> inks,<sup>3</sup> optical materials,<sup>4</sup> determination of proteins,<sup>5</sup> nucleic acid,<sup>6</sup> clay minerals<sup>7</sup>

**Safety/Toxicity** No data available

### References

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## MALACHITE GREEN

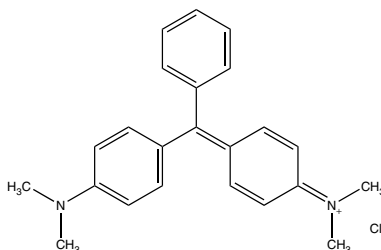
**Other Names** C.I. Basic Green 4; Victoria Green WB; ADC Malachite Green Crystals; Acryl Brilliant Green B; Aizen Malachite Green; Aizen Malachite Green Crystals; Aizen malachite green liquid; Aniline green; Astra Malachite Green; Astra Malachite Green B; Astra Malachite Green BXX; Atlantic Malachite Green; Basacryl Green X-BF; Basic Green 4; Basonyl Green 830; Basonyl Green NB 832; Benzal Green; Benzaldehyde green; Bronze Green Toner A 8002; Burma Green B; C.I. 42000; Calcozine Green V; China Green; Diabasic Malachite Green; Diamond Green B extra; Diamond Green BX; Diamond Green P Extra; Green MX; Green Malaquite; Grenoble Green; Hidaco Malachite Green Base; Hidaco Malachite Green LC; Hidaco Malachite Green SC; LC 6220; Light Green N; Lincoln Green Toner B 15-2900; Malachite Green 4; Malachite Green A; Malachite Green AN; Malachite Green B; Malachite Green CP; Malachite Green Crystals; Malachite Green Crystals BPC; Malachite Green J 3E; Malachite Green Powder; Malachite Green WS; Malachite Green XLS; Malachite Lake Green A; Malachite green; Malachite green chloride; Mitsui Malachite Green; New Victoria Green Extra I; New Victoria Green Extra II; New Victoria Green Extra O; Oji Malachite Green; Solid Green Crystals O; Solid Green O; Super Ick Cure; Tertrophenene Green M; Tokyo Aniline Malachite Green; Verona Basic Green M; Victoria Green; Victoria Green (basic dye); Victoria Green B; Victoria Green S; Victoria Green WPB

**CA Index Name** Methanaminium, *N*-[4-[[4-(dimethylamino)phenyl]-phenylmethylene]-2,5-cyclohexadien-1-ylidene]-*N*-methyl-, chloride

**CAS Registry Number** 569-64-2

**Merck Index Number** 5699

### Chemical Structure



**Chemical/Dye Class** Triphenylmethane

**Molecular Formula**  $C_{23}H_{25}N_2Cl$

**Molecular Weight** 364.92

**pH Range** 0.0–2.0;

11.6–14.0

**Color Change at pH** Yellow (0.0) to green (2.0)

Green (11.6) to colorless (14.0)

**pKa** 6.90

**Physical Form** Green crystals

**Solubility** Very soluble in water; soluble in ethanol, methanol, amyl alcohol

**UV-Visible** ( $\lambda_{max}$ ) 615 nm, 425 nm

**Melting Point** 112–114°C

**Synthesis** Synthetic methods<sup>1–13</sup>

**Major Applications** Photoresists,<sup>14</sup> color filter,<sup>15</sup> printed circuit board,<sup>16</sup> sol-gel matrix,<sup>17</sup> liquid crystal displays,<sup>18</sup> decoder system,<sup>19</sup> inks,<sup>20</sup> highlighters,<sup>21</sup> herbicides,<sup>22</sup> disinfectants,<sup>23</sup> cosmetics,<sup>25</sup> identifying mammal genes,<sup>25</sup> detecting nucleic acids,<sup>26</sup> mycobacterial growth,<sup>27</sup> multidrug resistance inhibitors,<sup>28</sup> radiochemotherapy,<sup>29</sup> wound dressing materials,<sup>30</sup> antitumor agents,<sup>31</sup> treatment of patients with pulmonary tuberculosis<sup>32</sup>

**Safety/Toxicity** Acute toxicity,<sup>33</sup> carcinogenicity,<sup>34</sup> cytotoxicity,<sup>35</sup> genotoxicity,<sup>36</sup> mutagenicity,<sup>37</sup> toxicological effects<sup>38</sup>

## References

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## MARTIUS YELLOW

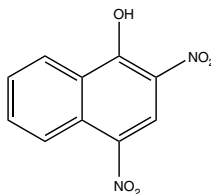
**Other Names** Acid Yellow 24; 1-Naphthol, 2,4-dinitro-; 1-Hydroxy-2,4-dinitronaphthalene; 2,4-Dinitro-1-naphthol; 2,4-Dinitronaphthol; Martinsgelb; Martius yellow; Manchester Yellow; NSC 6148

**CA Index Name** 1-Naphthalenol, 2,4-dinitro-

**CAS Registry Number** 605-69-6

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Nitro

**Molecular Formula** C<sub>10</sub>H<sub>6</sub>N<sub>2</sub>O<sub>5</sub>

**Molecular Weight** 234.16

**pH Range** 2.0–3.2

**Color Change at pH** Colorless (2.0) to yellow (3.2)

**pKa** 2.12

**Physical Form** Yellow orange powder

**Solubility** Very slightly soluble in water, ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 430 nm, 420 nm, 432 nm

**Melting Point** 138°C

**Boiling Point (Calcd.)** 407.9 ± 35.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–11</sup>

**Major Applications** Photoresists,<sup>12</sup> magnetic recording materials,<sup>13</sup> explosives,<sup>14</sup> polymerization inhibitor,<sup>15</sup> surface coatings,<sup>16</sup> coloring hair,<sup>17</sup> for animal identification<sup>18</sup>

**Safety/Toxicity** Toxicology,<sup>19</sup> toxicity,<sup>20,21</sup> mutagenicity<sup>22,23</sup>

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## MESALAMINE

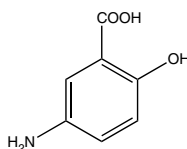
**Other Names** Salicylic acid, 5-amino-; 2-Hydroxy-5-aminobenzoic acid; 3-Carboxy-4-hydroxy-aniline; 5-ASA; 5-Amino-2-hydroxybenzoic acid; 5-Aminosalicylic acid; Asacol; Asacolitin; Asacolon; Canasa; Claversal; Fisasalmine; Ipocol; Lixacol; Mesacol; Mesalamine; Mesalazine; Mesasal; NSC 38877; Pentasa; Rowasa; Salofalk; Salozinal; *m*-Aminosalicylic acid

**CA Index Name** Benzoic acid, 5-amino-2-hydroxy-

**CAS Registry Number** 89-57-6

**Merck Index Number** 5904

### Chemical Structure



**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>7</sub>H<sub>7</sub>NO<sub>3</sub>

**Molecular Weight** 153.14

**pH Range** 3.1–4.4

**Color Change at pH** Nonfluorescence (3.1) to light green fluorescence (4.4)

**pKa** 2.74, 5.84

**Physical Form** White to pinkish crystals

**Solubility** Slightly soluble in cold water, ethanol; more soluble in hot water; soluble in hydrochloric acid

**Melting Point** 280°C (decompose)

**Boiling Point (Calcd.)** 403.9 ± 40.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–14</sup>

**Major Applications** Detergent,<sup>15</sup> hair dyes,<sup>16</sup> prevention of colorectal cancer,<sup>17</sup> treating inflammatory bowel disease,<sup>18</sup> autoimmune disorders,<sup>19</sup> gastrointestinal inflammation,<sup>20</sup> chemokine-mediated diseases,<sup>21</sup> mucosal tissue disorder,<sup>22</sup> sleep disorders,<sup>23</sup> rectoanal tenesmus,<sup>24</sup> ulcerative colitis<sup>25</sup>

**Safety/Toxicity** Hepatotoxicity,<sup>26,27</sup> cytotoxicity,<sup>27,28</sup> nephrototoxicity,<sup>29</sup> risk of renal disease,<sup>30</sup> safety in pregnancy,<sup>31</sup> side effects<sup>32</sup>

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## METANIL YELLOW

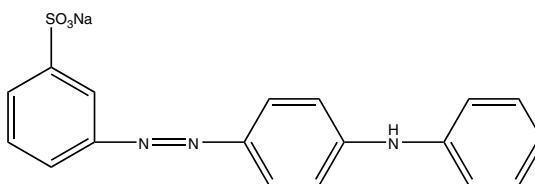
**Other Names** Benzenesulfonic acid, *m*-(*p*-anilinophenylazo)-, sodium salt; C.I. Acid Yellow 36; C.I. Acid Yellow 36, monosodium salt; 11363 Yellow; Acid Gold Yellow G; Acid Golden G; Acid Golden Yellow G; Acid Leather Yellow PRW; Acid Leather Yellow R; Acid Yellow 36; Acid Yellow Metanil; Aizen Metanil Yellow; Amacid Yellow M; Basacid Yellow 230; Basacid Yellow 232; Brasilan Metanil Yellow; Bucacid Metanil Yellow; C Ext. Yellow 10; C.I. 13065; Calcocid Yellow MXXX; Diacid Metanil Yellow; Egacid Yellow M; Egacid Yellow MA; Eniacid Metanil Yellow GN; Ext D & C Yellow 1; Ext D and C Yellow No. 1; Fenazo Yellow M; Hidacid Metanil Yellow; Hispacid Yellow MG; Japan Yellow 406; Japan Yellow No. 406; Java Metanil Yellow G; Kiton Orange MNO; Kiton Yellow MS; Metanil Yellow; Metanil Yellow 1955; Metanil Yellow C; Metanil Yellow E; Metanil Yellow Extra; Metanil Yellow F; Metanil Yellow G; Metanil Yellow Griesbach; Metanil Yellow K; Metanil Yellow KRSU; Metanil Yellow M; Metanil Yellow M 3X; Metanil Yellow O; Metanil Yellow PL; Metanil Yellow S; Metanil Yellow Supra P; Metanil Yellow VS; Metanil Yellow WS; Metanil Yellow Y; Metanil Yellow YK; Metanile Yellow O; Metanilic Yellow; Mitsui Metanil Yellow; Remaderm Yellow HPR; Shikiso Metanil Yellow; Sodium 4'-anilinoazobenzene-3-sulfonate; Sodium *m*-(4-anilinophenylazo)-benzenesulfonate; Sodium *m*-sulfonate-*p*-phenylazodiphenylamine; Symulon Metanil Yellow; Takaoka Metanil Yellow; Tertracid Yellow M; Tropaeolin G; Vondacid Metanil Yellow G; Yellow Methanil; Yellow No. 406; Yodochrome Metanil Yellow

**CA Index Name** Benzenesulfonic acid, 3-[[4-(phenylamino)phenyl]azo]-, monosodium salt

**CAS Registry Number** 587-98-4

**Merck Index Number** 5928

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>18</sub>H<sub>14</sub>N<sub>3</sub>O<sub>3</sub>SNa

**Molecular Weight** 375.38

**pH Range** 1.2–2.3

**Color Change at pH** Red (1.2) to yellow (2.3)

**Physical Form** Orange-red powder

**Solubility** Soluble in water, ethanol; moderately soluble in ether, benzene; slightly soluble in acetone, xylene

**UV-Visible** ( $\lambda_{\text{max}}$ ) 414 nm, 435 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1</sup>

**Major Applications** Display device,<sup>2</sup> nanoparticles,<sup>3</sup> optical sensors,<sup>4</sup> batteries,<sup>5</sup> lithographic printing plates,<sup>6</sup> inks,<sup>7</sup> highlighters,<sup>8</sup> children's coloring books,<sup>9</sup> floor coatings,<sup>10</sup> disinfectants,<sup>11</sup> hair dyes,<sup>12–14</sup> personal care products,<sup>15</sup> cosmetics,<sup>16</sup> food storage,<sup>17</sup> antiseptic,<sup>18</sup> dental impression materials<sup>19</sup>

**Safety/Toxicity** Acute toxicity,<sup>20</sup> carcinogenic effects,<sup>21</sup> hepatocarcinogenesis,<sup>22</sup> mutagenicity<sup>23,24</sup>

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## 2-METHOXYBENZALDEHYDE

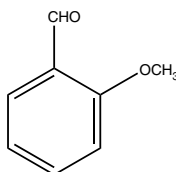
**Other Names** Benzaldehyde, *o*-methoxy-; *o*-Anisaldehyde; 2-Anisaldehyde; 2-Methoxybenzaldehyde; 2-Methoxybenzenecarboxaldehyde; 2-Methoxyphenylformaldehyde; 6-Methoxybenzaldehyde; NC 064; NSC 58960; Salicylaldehyde methyl ether; *o*-Formylanisole; *o*-Methoxybenzaldehyde

**CA Index Name** Benzaldehyde, 2-methoxy-

**CAS Registry Number** 135-02-4

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>8</sub>H<sub>8</sub>O<sub>2</sub>

**Molecular Weight** 136.15

**pH Range** 3.1–4.4

**Color Change at pH** Nonfluorescence (3.1) to green fluorescence (4.4)

**Physical Form** Off-white to light yellow crystals

**Solubility** Slightly soluble in water; soluble in ethanol

**Melting Point** 37–39°C

**Boiling Point** 238°C

**Synthesis** Synthetic methods<sup>1–6</sup>

**Major Applications** Battery,<sup>7,8</sup> hair dyes,<sup>9,10</sup> bird repellents,<sup>11,12</sup> cosmetics,<sup>13</sup> antibacterial,<sup>14</sup> anti-pyretic agent<sup>15</sup>

**Safety/Toxicity** Aquatic toxicity,<sup>16</sup> algae toxicity<sup>17</sup>

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## 4-METHYLESCULETIN

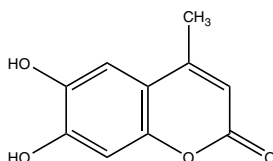
**Other Names** Coumarin, 6,7-dihydroxy-4-methyl-; Esculetin, 4-methyl-; 4-Methyl-6,7-dihydroxy-coumarin; 4-Methylaesculetin; 4-Methylesculetin; 4-Methylesculetol; 6,7-Dihydroxy-4-methyl-coumarin; Methylesculetin; NSC 11828; NSC 688807

**CA Index Name** 2H-1-Benzopyran-2-one, 6,7-dihydroxy-4-methyl-

**CAS Registry Number** 529-84-0

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Coumarin

**Molecular Formula** C<sub>10</sub>H<sub>8</sub>O<sub>4</sub>

**Molecular Weight** 192.17

**pH Range** 4.0–6.2

**Color Change at pH** Colorless (4.0) to blue fluorescent (6.2)

**pKa** 8.72

**Physical Form** Light brown powder

**Solubility** Very slightly soluble in water; slightly soluble in ethanol; soluble in ether, chloroform, ethylene glycol

**UV-Visible ( $\lambda_{\max}$ )** 348 nm, 292 nm

**Melting Point** 274–276°C

**Boiling Point (Calcd.)** 455.5 ± 45.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–9</sup>

**Major Applications** Electroluminescent device,<sup>10</sup> photoresists,<sup>11,12</sup> photography,<sup>13,14</sup> analytical reagent,<sup>15</sup> cosmetics,<sup>16–19</sup> hair dye,<sup>20–29</sup> shampoo,<sup>30,31</sup> antioxidant,<sup>32</sup> hypotensive agent,<sup>33</sup> antiinflammatory agent,<sup>34</sup> antiviral agent,<sup>35</sup> multidrug resistance (MDR) modulator,<sup>36</sup> inhibitory effect on melanin biosynthesis,<sup>37</sup> protective agent against DNA damage,<sup>38</sup> antimutagenic agent,<sup>39–41</sup> detection of tumor cell-specific cytotoxicity,<sup>42</sup> antiproliferative agent against cancer cells,<sup>43</sup> analysis of human pancreatic cancer cell activity,<sup>44</sup> chondroprotective agent<sup>45</sup>

**Safety/Toxicity** Chondroprotective agent<sup>45</sup>

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## METHYL GREEN

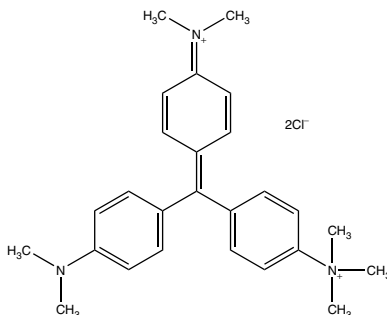
**Other Names** Methyl Green

**CA Index Name** Methyl Green

**CAS Registry Number** 54327-10-5

**Merck Index Number** Not listed

**Chemical Structure**



**Note:** The traditional Methyl Green has not manufactured for decades. The dye sold as Methyl Green is more accurately described as Ethyl Green. Both, Methyl Green and Ethyl Green are sold as double zinc salts.

**Chemical/Dye Class** Triphenylmethane

**Molecular Formula**  $C_{26}H_{33}N_3Cl_2$

**Molecular Weight** 458.46

**pH Range** 0.1–2.3

**Color Change at pH** Yellow (0.1) to greenish-blue (2.3)

**Physical Form** Green crystalline power

**Solubility** Soluble in water, ethanol; insoluble in xylene

**UV-Visible** ( $\lambda_{max}$ ) 635 nm, 420 nm

**Melting Point** >300°C

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Liquid crystal display device,<sup>3</sup> photography,<sup>4</sup> recording materials,<sup>5</sup> inks,<sup>6</sup> cosmetics,<sup>7</sup> DNA staining,<sup>8</sup> cancer detection<sup>9</sup>

**Safety/Toxicity** Toxicity to fresh water organisms<sup>10</sup>

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## METHYL ORANGE

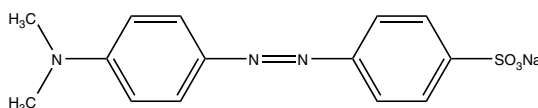
**Other Names** Benzenesulfonic acid, *p*-[[*p*-(dimethylamino)phenyl]azo]-, sodium salt; Orange III; 4-Dimethylaminoazobenzene-4'-sulfonic acid sodium salt; C.I. 13025; C.I. Acid Orange 52; Diazo-ben; Eniamethyl Orange; Gold orange; Helianthine; Helianthine B; KCA Methyl Orange; Methyl Orange B; Methyl orange; Orange 3; Sodium 4'-(dimethylamino)azobenzene-4-sulfonate; Sodium 4-(dimethylamino)azobenzene-4'-sulfonate; Sodium 4-[4-(dimethylamino)-phenylazo]-benzene-sulfonate; Sodium *p*-[*p*-(dimethylamino)-phenylazo]-benzenesulfonate; Sodium *p*-dimethylaminoazobenzenesulfonate; Tropaeolin D

**CA Index Name** Benzenesulfonic acid, 4-[[4-(dimethylamino)phenyl]azo]-, sodium salt

**CAS Registry Number** 547-58-0

**Merck Index Number** 6105

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>14</sub>H<sub>14</sub>N<sub>3</sub>O<sub>3</sub>SNa

**Molecular Weight** 327.34

**pH Range** 3.0–4.4

**Color Change at pH** Red (3.0) to yellow (4.4)

**pKa** 3.76, 3.40

**Physical Form** Orange powder

**Solubility** Slightly soluble in water, more soluble in hot water; practically insoluble in ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 507 nm, 522 nm, 464 nm

**Melting Point** >300°C

**Synthesis** Synthetic methods<sup>1–9</sup>

**Major Applications** Liquid crystals,<sup>10</sup> thin films,<sup>11</sup> sensors,<sup>12</sup> sol-gel matrix,<sup>13</sup> waveguides,<sup>14</sup> host-guest chemistry,<sup>15</sup> display device,<sup>16</sup> corrosion inhibitor,<sup>17</sup> glass coatings,<sup>18</sup> paints,<sup>19</sup> wound dressing materials,<sup>20</sup> pharmaceuticals,<sup>21</sup> dental materials,<sup>22</sup> measuring nucleic acid<sup>23</sup>

**Safety/Toxicity** Carcinogenicity,<sup>24</sup> genotoxicity,<sup>25</sup> mutagenicity<sup>26</sup>

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## METHYL PURPLE

**Other Names** Fleisher's Methyl purple indicator

**CA Index Name** Methyl purple

**CAS Registry Number** 1340-02-9

**Merck Index Number** Not listed

**Chemical Structure** No structure diagram available

**Chemical/Dye Class** No data available

**Molecular Formula** Unspecified

**Molecular Weight** No data available

**pH Range** 4.8–5.4

**Color Change at pH** Purple (4.8) to green (5.4)

**pKa** No data available

**Physical Form** Green powder

**Solubility** Soluble in water, ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 410 nm, 620 nm

**Melting Point** Not available

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Analysis of selenium in marine organisms,<sup>2,3</sup> detecting lactic acid bacteria,<sup>4</sup> determination of iron in human hair,<sup>5</sup> antimicrobial agent<sup>6</sup>

**Safety/Toxicity** No data available

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## METHYL RED

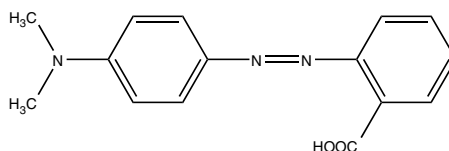
**Other Names** C.I. Acid Red 2; 2-Carboxy-4'-(dimethylamino)azobenzene; 2-[(*p*-Dimethylamino)-phenyl]azobenzoic acid; 2-[[4-(Dimethylamino)-phenyl]azo]benzoic acid; 4'-(Dimethylamino)-azobenzene-2-carboxylic acid; 4-(2-Carboxyphenylazo)-*N,N*-dimethylaniline; Acid Red 2; C.I. 13020; Methyl red; Methyl red C.I. 13020; NSC 215212; NSC 34729; NSC 9597; *o*-Methyl red; *o*-[[*p*-(Dimethylamino)-phenyl]azo]-benzoic acid; *p*-(Dimethylamino)-azobenzene-*o*-carboxylic acid

**CA Index Name** Benzoic acid, 2-[[4-(dimethylamino)phenyl]azo]-

**CAS Registry Number** 493-52-7

**Merck Index Number** 6119

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>15</sub>H<sub>15</sub>N<sub>3</sub>O<sub>2</sub>

**Molecular Weight** 269.30

**pH Range** 4.4–6.2

**Color Change at pH** Red (4.4) to yellow (6.2)

**pKa** 5.06, 2.3, 2.5, 4.95

**Physical Form** Maroon-red crystals

**Solubility** Almost insoluble in water; soluble in ethanol, acetic acid

**UV-Visible** ( $\lambda_{\text{max}}$ ) 410 nm, 530 nm, 427 nm, 519 nm

**Melting Point** 181–182°C

**Boiling Point (Calcd.)** 479.5 ± 30.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–4</sup>

**Major Applications** Waveguides,<sup>5</sup> LED sensors,<sup>6</sup> photoresists,<sup>7</sup> liquid crystals,<sup>8</sup> sol-gel matrix,<sup>9</sup> optical sensors,<sup>10</sup> paints,<sup>11</sup> toys,<sup>12</sup> detection of thiols,<sup>13</sup> food freshness sensors,<sup>14</sup> dental product,<sup>15</sup> saliva sampling method,<sup>16</sup> detecting lactic acid,<sup>17</sup> carbohydrates<sup>18</sup>

**Safety/Toxicity** Carcinogenicity,<sup>19</sup> genotoxicity,<sup>20</sup> mutagenicity<sup>21</sup>

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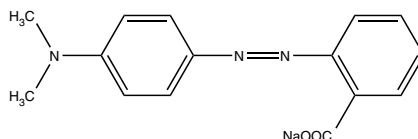
**METHYL RED, SODIUM SALT**

**Other Names** C.I. Acid Red 2, sodium salt; Methyl red sodium salt; *o*-Methyl red sodium salt

**CA Index Name** Benzoic acid, 2-[[4-(dimethylamino)phenyl]azo]-, sodium salt

**CAS Registry Number** 845-10-3

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>15</sub>H<sub>14</sub>N<sub>3</sub>O<sub>2</sub>Na

**Molecular Weight** 291.29

**pH Range** 1.2–3.4;

4.2–6.3

**Color Change at pH** Red (1.2) to orange (3.4)

Red (4.2) to yellow (6.3)

**pKa** 2.3, 5.0

**Physical Form** Orange powder

**Solubility** Soluble in water, ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 437 nm, 410 nm, 493 nm

**Melting Point** >300°C

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Optical filters,<sup>3,4</sup> liquid crystal cells,<sup>5,6</sup> holography,<sup>7,8</sup> inks,<sup>9</sup> toner,<sup>10</sup> corrosion inhibitor,<sup>11</sup> detergent<sup>12</sup>

**Safety/Toxicity** No data available

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## 4-METHYUMBELLIFERONE

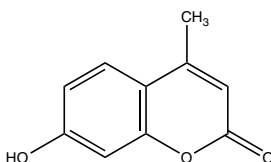
**Other Names** Coumarin, 7-hydroxy-4-methyl-; Umbelliferone, 4-methyl-;  $\beta$ -Methylumbelliferone; 4-MU; 4-Methyl-7-hydroxycoumarin; 4-Methylumbelliferone; 7-Hydroxy-4-methyl-2-chromenone; 7-Hydroxy-4-methyl-2-oxo-3-chromene; 7-Hydroxy-4-methyl-2H-1-benzopyran-2-one; 7-Hydroxy-4-methyl-2H-chromen-2-one; 7-Hydroxy-4-methylcoumarin; Bilcolic; Bilicante; Biliton H; Cantabilin; Cantabiline; Cholestil; Cholonerton; Cholspasmin; Coumarin 4; Coumarin 456; Cumarote C; Eurogale; Himecol; Hymecromone; Imecromone; LM 94; Medilla; Mendiaxon; NSC 19026; NSC 9408; Omega 127; Pilot 447

**CA Index Name** 2H-1-Benzopyran-2-one, 7-hydroxy-4-methyl-

**CAS Registry Number** 90-33-5

**Merck Index Number** 4854

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Coumarin

**Molecular Formula**  $C_{10}H_8O_3$

**Molecular Weight** 176.17

**pH Range** 0.0–2.0;

6.5–8.0

**Color Change at pH** Green fluorescent (0.0) to weak blue fluorescent (2.0)

Weak blue fluorescent (6.5) blue fluorescent (8.0)

**pKa** 7.79

**Physical Form** White to off-white powder

**Solubility** Practically insoluble in water; slightly soluble in ethanol, ether, chloroform; soluble in methanol

**UV-Visible ( $\lambda_{\max}$ )** 221 nm, 251 nm, 322 nm

**Melting Point** 194–195°C

**Boiling Point (Calcd.)**  $377.4 \pm 37.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–15</sup>

**Major Applications** Color filter,<sup>16</sup> electroluminescent displays,<sup>17</sup> document security processes,<sup>18</sup> lasers,<sup>19</sup> integrated circuits,<sup>20</sup> liquid crystal displays,<sup>21</sup> surface brightening composition,<sup>22</sup> oil products,<sup>23</sup> teeth whitening agent,<sup>24</sup> lysosomal enzyme assay,<sup>25</sup> substrate for lipase,<sup>26</sup> determining protein-protein-interactions in living cells,<sup>27</sup> Antitrypanosomal,<sup>28</sup> antileishmanial,<sup>28</sup> anticancer,<sup>29</sup> antiHIV,<sup>30</sup> antimalarial,<sup>31</sup> antibacterial,<sup>32</sup> antifungal<sup>32</sup>

**Safety/Toxicity** Acute oral toxicity,<sup>33</sup> ecotoxicology,<sup>34</sup> human health effects,<sup>35</sup> mutagenicity<sup>36</sup>

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## METHYL VIOLET

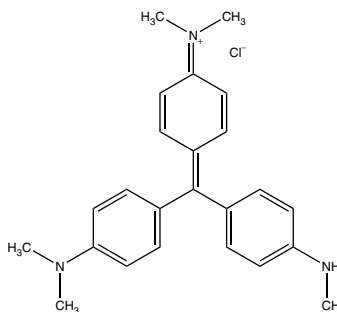
**Other Names** Methyl Violet; Aizen Methyl Violet BB; Aizen Methyl Violet Pure Special; Basic Violet 1; Basic Violet 5BN; Basic Violet K; Basonyl Violet 600; C Ext. Violet 5; C.I. 42535; Gentian Violet B; Methyl Violet 2B; Methyl Violet 6B; Methyl Violet B; Methyl Violet BB; Methyl Violet FN; Methyl Violet N; Methyl Violet Pure Special; Methyl Violet pure SP; Paris Violet R; Pyoktanin blue; Pyoktaninum coeruleum; Violet Powder H 2503

**CA Index Name** C.I. Basic Violet 1

**CAS Registry Number** 8004-87-3

**Merck Index Number** Not listed

**Chemical Structure** It is a mixture of *N*-pentamethyl (as shown) and *N*-hexamethyl (which is Crystal Violet) *p*-rosaniline chlorides



**Chemical/Dye Class** Triphenylmethane

**Molecular Formula** Mixture of tetra-, penta-, & hexamethyl *p*-rosaniline chlorides

**Molecular Weight** Mixture of tetra-, penta-, & hexamethyl *p*-rosaniline chlorides

**pH Range** 0.15–3.2

**Color Change at pH** Yellow (0.15) to violet (3.2)

**Physical Form** Green crystals

**Solubility** Soluble in water, ethanol, chloroform; insoluble in ether, xylene

**UV-Visible ( $\lambda_{\text{max}}$ )** 584 nm

**Melting Point** 137°C (decompose)

**Synthesis** Synthetic methods<sup>1–6</sup>

**Major Applications** Display device,<sup>7,8</sup> photoresists,<sup>9</sup> solar cells,<sup>10</sup> inks,<sup>11,12</sup> highlighters,<sup>13</sup> rubber,<sup>14</sup> lithium battery,<sup>15</sup> petroleum products,<sup>16</sup> leak detection method,<sup>17</sup> decoder system,<sup>18</sup> packaging materials,<sup>19</sup> hair dyes,<sup>20</sup> cosmetics,<sup>21</sup> wound dressing materials,<sup>22</sup> antitumor agent,<sup>23</sup> determination of nucleic acids<sup>24</sup>

**Safety/Toxicity** Acute toxicity,<sup>25</sup> carcinogenicity,<sup>26</sup> toxicity to aquatic microbes,<sup>27</sup> mutagenicity<sup>28</sup>

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## METHYL YELLOW

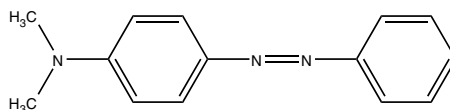
**Other Names** Aniline, *N,N*-dimethyl-*p*-phenylazo-; Butter yellow; C.I. Solvent Yellow 2; (4-Dimethylaminophenyl)phenyldiazene; (*p*-Dimethylaminophenyl)phenyldiazene; 4-(Dimethylamino)-azobenzene; 4-(*N,N*-Dimethylamino)azobenzene; 4-(Phenylazo)-*N,N*-dimethylaniline; Brilliant Fast Oil Yellow; Brilliant Fast Spirit Yellow; Brilliant Oil Yellow; C.I. 11020; Cerasine Yellow GG; DAB; DAB (carcinogen); DMAB; Dimethyl Yellow; Enial Yellow 2G; Fast Oil Yellow B; Fat Yellow; Fat Yellow A; Fat Yellow AD OO; Fat Yellow ES; Fat Yellow ES Extra; Fat Yellow R; Fat Yellow extra conc; Grasal Brilliant Yellow; Iketon Yellow Extra; Methyl yellow; *N,N*-Dimethyl-4-(phenylazo)aniline; *N,N*-Dimethyl-*p*-(phenylazo)aniline; NSC 6236; Oil Yellow 20; Oil Yellow 2625; Oil Yellow 2G; Oil Yellow BB; Oil Yellow D; Oil Yellow FN; Oil Yellow G; Oil Yellow GG; Oil Yellow GR; Oil Yellow II; Oil Yellow N; Oil Yellow PEL; Oil Yellow S; Oleal Yellow 2G; Organol Yellow ADM; Orient Oil Yellow GG; Petrol Yellow WT; Resinol Yellow GR; Silotras Yellow T 2G; Somalia Yellow A; Stear Yellow JB; Sudan Yellow GG; Sudan Yellow GGA; Toyo Oil Yellow G; Waxoline Yellow ADS; Yellow G Soluble in Grease; *p*-(Dimethylamino)azobenzene

**CA Index Name** Benzenamine, *N,N*-dimethyl-4-(phenylazo)-

**CAS Registry Number** 60-11-7

**Merck Index Number** 3229

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{14}H_{15}N_3$

**Molecular Weight** 225.29

**pH Range** 2.9-4.0

**Color Change at pH** Red (2.9) to yellow (4.0)

**pKa** 3.3, 3.4

**Physical Form** Orange-yellow powder

**Solubility** Insoluble in water; soluble in ethanol, benzene, ether, chloroform, petroleum ether, mineral acids, oils

**UV-Visible ( $\lambda_{max}$ )** 408 nm, 256 nm, 508 nm

**Melting Point** 114–117°C

**Boiling Point (Calcd.)**  $371.1 \pm 25.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1-8</sup>

**Major Applications** Electrochromic materials,<sup>9</sup> sol-gel coatings,<sup>10</sup> display device,<sup>11</sup> inks,<sup>12</sup> gas detection apparatus,<sup>13</sup> nematocides,<sup>14</sup> hair dyes,<sup>15</sup> diapers,<sup>16</sup> food storage,<sup>17</sup> status assessment in breast cancer,<sup>18</sup> detecting carbohydrates,<sup>19</sup> bacteria,<sup>20</sup> diagnosing cervical disease,<sup>21</sup> wound dressing materials<sup>22</sup>

**Safety/Toxicity** Cytotoxicity,<sup>23</sup> carcinogenicity,<sup>24</sup> mutagenicity<sup>25</sup>

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# N

## $\alpha$ -NAPHTHOIC ACID

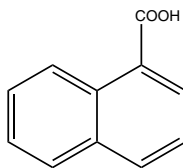
**Other Names** 1-Naphthoic acid;  $\alpha$ -Naphthoic acid;  $\alpha$ -Naphthylcarboxylic acid; 1-Carboxynaphthalene; 1-Naphthylcarboxylic acid; NSC 37569; Naphthalene- $\alpha$ -carboxylic acid

**CA Index Name** 1-Naphthalenecarboxylic acid

**CAS Registry Number** 86-55-5

**Merck Index Number** 6381

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Naphthalene

**Molecular Formula**  $C_{11}H_8O_2$

**Molecular Weight** 172.18

**pH Range** 2.5–3.5

**Color Change at pH** Nonfluorescence (2.5) to blue fluorescence (3.5)

**pKa** 3.68

**Physical Form** Colorless crystals

**Solubility** Slightly soluble in hot water; freely soluble in hot ethanol, ether

**UV-Visible ( $\lambda_{\max}$ )** 293 nm

**Melting Point** 161°C

**Boiling Point** 300°C

**Synthesis** Synthetic methods<sup>1–13</sup>

**Major Applications** Photoresists,<sup>14</sup> recording materials,<sup>15</sup> waveguides,<sup>16</sup> battery,<sup>17</sup> ink,<sup>18</sup> rubber,<sup>19,20</sup> plastic films,<sup>21</sup> agriculture,<sup>22</sup> cosmetics,<sup>23</sup> sunscreens,<sup>24</sup> method for preserving food,<sup>25</sup> drugs,<sup>26</sup> biosensors<sup>27</sup>

**Safety/Toxicity** Acute toxicity,<sup>28</sup> skin corrosivity<sup>29</sup>

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## $\beta$ -NAPHTHOL

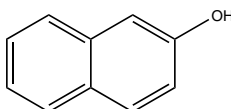
**Other Names** 2-Naphthol;  $\beta$ -Hydroxynaphthalene;  $\beta$ -Naphthol;  $\beta$ -Naphthyl alcohol; 2-Hydroxynaphthalene; Azogen Developer A; Betanaphthol; C.I. 37500; C.I. Azoic Coupling Component 1; C.I. Developer 5; Developer A; Developer AMS; Developer BN; Developer NA; Isonaphthol; NSC 2044; NSC 5737; Naphthol B

**CA Index Name** 2-Naphthalenol

**CAS Registry Number** 135-19-3

**Merck Index Number** 6384

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Naphthalene

**Molecular Formula**  $C_{10}H_8O$

**Molecular Weight** 144.17

**pH Range** 8.5–9.5

**Color Change at pH** Nonfluorescence (8.5) to blue fluorescence (9.5)

**pKa** 9.57

**Physical Form** Buff crystals

**Solubility** Very slightly soluble in water; soluble in ethanol, ether, glycerin

**UV-Visible** ( $\lambda_{max}$ ) 226 nm, 265 nm, 275 nm, 286 nm, 320 nm, 331 nm

**Melting Point** 120–123°C

**Boiling Point** 285–286°C

**Synthesis** Synthetic methods<sup>1–13</sup>

**Major Applications** Display device,<sup>14</sup> semiconductors,<sup>15</sup> photoimaging materials,<sup>16</sup> inks,<sup>17</sup> toner,<sup>18</sup> chalk,<sup>19</sup> security paper,<sup>20</sup> molding materials,<sup>21</sup> tin plating method,<sup>22</sup> rubber,<sup>23</sup> adhesive,<sup>24</sup> leather,<sup>25</sup> detergent,<sup>26</sup> hair dyes,<sup>27</sup> antimitotic drug,<sup>28</sup> anticancer agent,<sup>29</sup> antiinflammatory agent,<sup>30</sup> treatment of acne vulgaris (pimples)<sup>31</sup> and other dermal ailments (rashes, scratches, blemishes, hair loss),<sup>31</sup> neurological disorders<sup>32</sup>

**Safety/Toxicity** Acute toxicity,<sup>33</sup> skin corrosivity,<sup>34</sup> cytotoxicity,<sup>35</sup> carcinogenicity,<sup>36</sup> aquatic toxicity,<sup>37</sup> ecotoxicity,<sup>38</sup> immunotoxicity,<sup>39</sup> environmental toxicity,<sup>40</sup> mutagenicity,<sup>41</sup> phytotoxicity<sup>42</sup>

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## NAPHTHOL AS

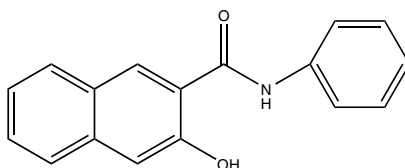
**Other Names** 2-Naphthanilide, 3-hydroxy-;  $\alpha$ -Naphthol AS; 2-Hydroxy-3-(phenylcarbamoyl)naphthalene; 2-Hydroxy-3-naphthalenecarboxanilide; 2-Hydroxy-3-naphthanilide; 2-Hydroxy-3-naphthoic acid anilide; 2-Hydroxy-3-naphthoic anilide; 2-Hydroxy-N-phenyl-3-naphthalenecarboxamide; 2-Naphthol-3-carboxylic acid N-phenylamide; 3-(N-Phenylcarbamoyl)-2-naphthol; 3-Hydroxy-2-naphthalenecarboxanilide; 3-Hydroxy-2-naphthanilide; 3-Hydroxy-2-naphthoic acid anilide; 3-Hydroxy-N-phenyl-2-naphthalenecarboxamide; 3-Hydroxy-N-phenyl-2-naphthamide; 3-Hydroxyl-2-naphthanilide; Acco Naphthol AS; Acna Naphthol C; Amanil Naphthol AS; Amarthol AS; Anthonaphthol AS; Aquafine Red E 9; Azoground AS; Azoic Coupling Component 2; Azonaphtol A; Azotol A; Brenthol AS; C.I. 37505; C.I. Azoic Coupling Component 2; Celcot RF; Cibanaphthol RF; Diathol AS; Diathol ASF; Dragonthol A; Hiltonaphthol AS; Kako Grounder AS; Kambothol AS; Lake Developer A; Mitsui Naphthozol AS; N-Phenyl-2-hydroxy-3-naphthalenecarboxamide; NSC 45173; Naftolo MM; Naphtanilide OL Supra; Naphtanilide RC; Naphtanilide RC Supra; Naphtazol A; Naphthanil AS; Naphthoide AS; Naphthoide AS No. 100; Naphthol ACNA C; Naphthol AS; Naphthol AS Supra; Naphthol AS-A; Naphtholate AS; Naphtoelan A; Naphtol AS; Solunaphtol A; Tulathol AS; Ultrazol I-AS

**CA Index Name** 2-Naphthalenecarboxamide, 3-hydroxy-*N*-phenyl-

**CAS Registry Number** 92-77-3

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Naphthalene

**Molecular Formula**  $C_{17}H_{13}NO_2$

**Molecular Weight** 263.29

**pH Range** 8.2–10.3

**Color Change at pH** Nonfluorescence (8.2) to yellow/green fluorescence (10.3)

**pKa** 9.70

**Physical Form** Beige powder

**Solubility** Insoluble in water; sparingly soluble in ethanol

**UV-Visible** ( $\lambda_{\max}$ ) 394 nm

**Melting Point** 247–250°C

**Boiling Point (Calcd.)**  $391.8 \pm 25.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–11</sup>

**Major Applications** Sensors,<sup>12</sup> recording materials,<sup>13</sup> photovoltaic cells,<sup>14</sup> copying materials,<sup>15</sup> photoreceptors,<sup>16</sup> lithographic printing plates,<sup>17</sup> inks,<sup>18</sup> toner,<sup>19</sup> paints,<sup>20</sup> textiles,<sup>21,22</sup> detecting cancer<sup>23</sup>

**Safety/Toxicity** Oral acute toxicity,<sup>24</sup> acute contact dermatitis<sup>25</sup>

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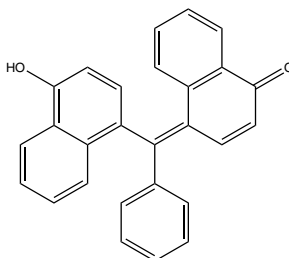
**$\alpha$ -NAPHTHOLBENZEIN**

**Other Names** 1(4H)-Naphthalenone, 4-[ $\alpha$ -(4-hydroxy-1-naphthyl)benzylidene]-;  $\alpha$ -Naphtholbenzein; NSC 9862; *p*-Naphtholbenzein

**CA Index Name:** 1(4H)-Naphthalenone, 4-[(4-hydroxy-1-naphthalenyl)-phenylmethylene]-

**CAS Registry Number** 145-50-6

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Benzein

**Molecular Formula**  $C_{27}H_{18}O_2$

**Molecular Weight** 374.43

**pH Range** 0.0-0.8;

8.2-11.0

**Color Change at pH** Green (0.0) to yellow (0.8)

Yellow (8.2) to green-blue (11.0)

**pKa** 8.95

**Physical Form** Red-brown powder

**Solubility** Insoluble in water; soluble in ethanol, methanol

**UV-Visible ( $\lambda_{\max}$ )** 210 nm

**Melting Point** 230-235°C

**Boiling Point (Calcd.)**  $578.6 \pm 50.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1-3</sup>

**Applications** Semiconducting polymers,<sup>4</sup> concrete,<sup>5</sup> correction fluid,<sup>6</sup> food storage,<sup>7</sup> determining bacterial growth in packed food,<sup>8</sup> personal hygiene products,<sup>9</sup> detecting viable cells,<sup>10</sup> detecting enzymes,<sup>11</sup> detecting ammonia odors in patients having bacterial infection<sup>12</sup>

**Safety/Toxicity** Acute oral toxicity<sup>13</sup>

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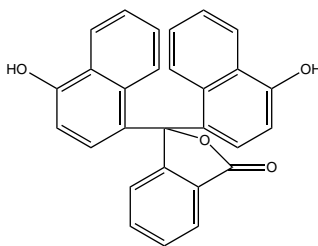
**$\alpha$ -NAPHTHOLPHTHALEIN**

**Other Names** 1,1'-Naphthol-4,4'-phthalein; Phthalide, 3,3-bis(4-hydroxy-1-naphthyl)-;  $\alpha$ -Naphtholphthalein; 1-Naphtholphthalein; 3,3-Bis(4-hydroxy-1-naphthyl)-1,3-dihydroisobenzofuran-1-one; 3,3-Bis(4-hydroxy-1-naphthyl)phthalide; Di-*p*- $\alpha$ -Naphtholphthalide; Naphtholphthalein blue; *p*- $\alpha$ -Naphtholphthalein

**CA Index Name** 1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxy-1-naphthalenyl)-

**CAS Registry Number** 596-01-0

**Merck Index Number** 6389

**Chemical Structure**

**Chemical/Dye Class** Phthalein

**Molecular Formula**  $C_{28}H_{18}O_4$

**Molecular Weight** 418.44

**pH Range** 7.3–8.7

**Color Change at pH** Colorless (7.3) to greenish-blue (8.7)

**pKa** 8.0, 8.2, 8.5

**Physical Form** Colorless powder when pure, usually grayish-red powder

**Solubility** Practically insoluble in water; soluble in ethanol

**UV-Visible ( $\lambda_{max}$ )** 648 nm

**Melting Point** 253–255°C

**Boiling Point (Calcd.)**  $705.6 \pm 60.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Applications** Sensors,<sup>3,4</sup> sol-gel materials,<sup>5</sup> thermochromic materials,<sup>6</sup> recording materials,<sup>7</sup> imaging materials,<sup>8</sup> authentication system for secure documents,<sup>9</sup> inks,<sup>10</sup> markers,<sup>11</sup> toners,<sup>12</sup> paints,<sup>13</sup> adhesives,<sup>14</sup> rubber,<sup>15</sup> lubricants,<sup>16</sup> food storage,<sup>17</sup> fruits or vegetable packaging,<sup>18</sup> detecting viable cells,<sup>19</sup> drugs,<sup>20</sup> oral hygiene products,<sup>21</sup> dental materials<sup>22</sup>

**Safety/Toxicity** No data available

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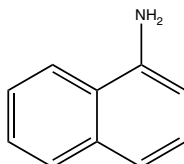
**$\alpha$ -NAPHTHYLAMINE**

**Other Names** 1-Naphthylamine;  $\alpha$ -Aminonaphthalene;  $\alpha$ -Naphthylamine; 1-Aminonaphthalene; 1-Naphthalamine; C.I. 37265; C.I. Azoic Diazo Component 114; Fast Garnet Base B; Naphthalen-1-ylamine; Naphthalidam; Naphthalidine

**CA Index Name** 1-Naphthalenamine

**CAS Registry Number** 134-32-7

**Merck Index Number** 6398

**Chemical Structure**

**Chemical/Dye Class** Fluorescent

**Molecular Formula**  $C_{10}H_9N$

**Molecular Weight** 143.19

**pH Range** 3.4–4.8

**Color Change at pH** Nonfluorescence (3.4) to blue fluorescence (4.8)

**pKa** 3.94

**Physical Form** Reddish needles

**Solubility** Slightly soluble in water; freely soluble in ethanol, ether

**Melting Point** 50°C

**Boiling Point** 301°C

**Synthesis** Synthetic methods<sup>1–12</sup>

**Major Applications** Color filter,<sup>13</sup> photoresists,<sup>14</sup> recording media,<sup>15</sup> light-emitting device,<sup>16</sup> optical disk,<sup>17</sup> display device,<sup>18</sup> oil products,<sup>19</sup> construction materials,<sup>20</sup> leather,<sup>21</sup> textile,<sup>22</sup> chalk,<sup>23</sup> detecting explosives<sup>24</sup>

**Safety/Toxicity** Carcinogenicity,<sup>25</sup> chemical toxicity,<sup>26</sup> genotoxicity,<sup>27</sup> hepatotoxicity,<sup>28</sup> mutagenicity,<sup>29</sup> phytotoxicity<sup>30</sup>

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## $\beta$ -NAPHTHYLAMINE

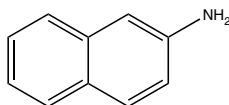
**Other Names** 2-Naphthylamine;  $\beta$ -Aminonaphthalene;  $\beta$ -Naphthylamine; 2-Aminonaphthalene; C.I. 37270; Fast Scarlet Base B; Naphthalen-2-ylamine; *o*-Aminonaphthalene

**CA Index Name** 2-Naphthalenamine

**CAS Registry Number** 91-59-8

**Merck Index Number** 6399

**Chemical Structure**



**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>10</sub>H<sub>9</sub>N

**Molecular Weight** 143.19

**pH Range** 2.8–4.4

**Color Change at pH** Nonfluorescence (2.8) to violet fluorescence (4.4)

**pKa** 4.20

**Physical Form** White to reddish crystals

**Solubility** Soluble in hot water, ethanol, ether

**Melting Point** 111–113°C

**Boiling Point** 306°C

**Synthesis** Synthetic methods<sup>1–4</sup>

**Major Applications** Microelectronics,<sup>5</sup> power transmission fluid,<sup>6</sup> insulators for electronic devices,<sup>7</sup> photoresists,<sup>8</sup> display device,<sup>9</sup> imaging process,<sup>10</sup> semiconductors,<sup>11</sup> diesel fuel additives,<sup>12</sup> battery,<sup>13</sup> adhesive,<sup>14</sup> paints,<sup>15</sup> inks,<sup>16</sup> chalk,<sup>17</sup> leather,<sup>18</sup> textiles,<sup>18</sup> dye synthesis,<sup>19</sup> soil products<sup>20</sup>

**Safety/Toxicity** Carcinogenicity,<sup>21,22</sup> cytotoxicity,<sup>23</sup> genotoxicity,<sup>23</sup> mutagenicity,<sup>24</sup> tumorigenicity<sup>25</sup>

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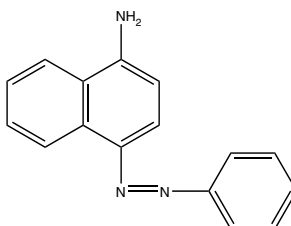
**$\alpha$ -NAPHTHYL RED**

**Other Names** 1-Naphthylamine, 4-phenylazo-; C.I. Solvent Yellow 4;  $\alpha$ -Naphthyl red; 4-(Phenylazo)- $\alpha$ -naphthylamine; 4-(Phenylazo)-1-naphthylamine; 4-Benzeneazo-1-naphthylamine; C.I. 11350; NSC 13974; Nubian Yellow TB

**CA Index Name** 1-Naphthalenamine, 4-(phenylazo)-

**CAS Registry Number** 131-22-6

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{16}H_{13}N_3$

**Molecular Weight** 247.29

**pH Range** 3.7–5.0

**Color Change at pH** Red (3.7) to yellow (5.0)

**pKa** 2.70

**Physical Form** Dark red crystals

**Solubility** Virtually insoluble in water; slightly soluble in ethanol; soluble in acetone, benzene, ethyl acetate, toluene, xylene

**UV-Visible ( $\lambda_{\max}$ )** 439 nm

**Melting Point** 124°C

**Boiling Point (Calcd.)**  $451.4 \pm 20.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–4</sup>

**Major Applications** Display device,<sup>5</sup> semiconductor,<sup>6</sup> sensors,<sup>7</sup> photosensitive materials,<sup>8</sup> recording materials,<sup>9</sup> imaging materials,<sup>10</sup> inks,<sup>11</sup> engraving coatings,<sup>12</sup> lubricants,<sup>13</sup> hair dyes,<sup>14</sup> food storage,<sup>15,16</sup> dental materials<sup>17,18</sup>

**Safety/Toxicity** oral toxicity,<sup>19</sup> mutagenicity<sup>20</sup>

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## NEUTRAL RED

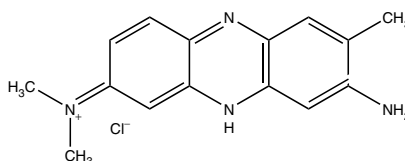
**Other Names** C.I. Basic Red 5, monohydrochloride; Toluylene red; 3-Amino-7-dimethylamino-2-methylphenazine hydrochloride; C.I. 50040; C.I. Basic Red 5; Neutral Red; Neutral Red W; Nuclear Fast Red (basic dye)

**CA Index Name** 2,8-Phenazinediamine, N8,N8,3-trimethyl-, monohydrochloride

**CAS Registry Number** 553-24-2

**Merck Index Number** 6488

### Chemical Structure



**Chemical/Dye Class** Miscellaneous, Azine

**Molecular Formula** C<sub>15</sub>H<sub>16</sub>N<sub>4</sub>.HCl

**Molecular Weight** 288.78

**pH Range** 6.8–8.0

**Color Change at pH** Red (6.8) to yellow (8.0)

**pKa** 6.7, 7.4

**Physical Form** Dark green or brownish-black powder

**Solubility** Soluble in water, ethanol; practically insoluble in xylene

**UV-Visible** ( $\lambda_{\text{max}}$ ) 540 nm, 533 nm, 544 nm, 529 nm, 454 nm

**Melting Point** 290°C (decompose)

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Fuel cell power generation system,<sup>6</sup> liquid crystal displays,<sup>7</sup> solar cells,<sup>8</sup> sensors,<sup>9</sup> thermochromic materials,<sup>10</sup> coloring wood,<sup>11</sup> detergents,<sup>12</sup> assessment of tobacco smoke,<sup>13</sup> cosmetics,<sup>14</sup> detect bacterial infections,<sup>15</sup> multidrug resistance inhibitors,<sup>16</sup> treatment of burns,<sup>17</sup> endodontic,<sup>18</sup> diabetes,<sup>19</sup> obesity,<sup>19</sup> cancer,<sup>20</sup> age-related macular degeneration,<sup>21</sup> viral diseases<sup>22</sup>

**Safety/Toxicity** Acute toxicity,<sup>23</sup> combustion toxicity,<sup>24</sup> cytotoxicity,<sup>25</sup> genotoxicity,<sup>26</sup> mutagenicity,<sup>27</sup> nephrotoxicity,<sup>28</sup> phototoxicity,<sup>29</sup> soil toxicity<sup>30</sup>

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## NILE BLUE

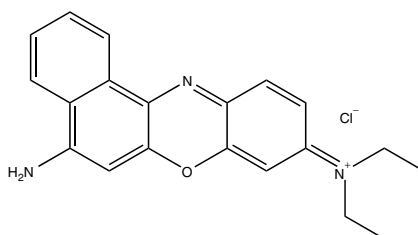
**Other Names** C.I. Basic Blue 12; Nile Blue; C.I. 51180; Cresol Fast Violet; Cresyl Fast Violet; Nile Blue AX; Nile Blue BX; Nile blue base; Nile blue chloride

**CA Index Name** Benzo[a]phenoxazin-7-ium, 5-amino-9-(diethylamino)-, chloride

**CAS Registry Number** 2381-85-3

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Miscellaneous, Oxazine

**Molecular Formula** C<sub>20</sub>H<sub>20</sub>N<sub>3</sub>OCl

**Molecular Weight** 353.85

**pH Range** 9.4–11.0

**Color Change at pH** Blue (9.4) to purple-red (11.0)

**pKa** 9.7

**Physical Form** Green powder

**Solubility** Soluble in water, ethanol

**UV-Visible (λ<sub>max</sub>)** 638 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** CMOS technology,<sup>4</sup> waveguides,<sup>5</sup> electroluminescent device,<sup>6</sup> inks,<sup>7</sup> plastics,<sup>8</sup> biofuel cells,<sup>9</sup> detect bacterial growth,<sup>10</sup> lipids,<sup>11</sup> DNA,<sup>12</sup> diagnosis of diseases related to amyloid accumulation,<sup>13</sup> fluorescent probes,<sup>14</sup> therapy of viral diseases,<sup>15</sup> photodynamic therapy<sup>16</sup>

**Safety/Toxicity** Carcinogenicity,<sup>17</sup> cytotoxicity,<sup>18</sup> mutagenicity,<sup>19</sup> teratogenicity<sup>20</sup>

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## NITRAMINE

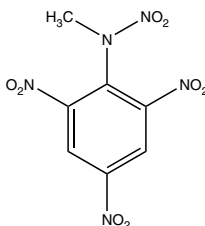
**Other Names** Aniline, *N*-methyl-*N*,2,4,6-tetranitro-; 2,4,6-*N*-Tetranitro-*N*-methylaniline; 2,4,6-Tetryl; 2,4,6-Trinitro-*N*-methyl-*N*-nitroaniline; 2,4,6-Trinitrophenyl-*N*-methylnitramine; 2,4,6-Trinitrophenylmethylnitroamine; CE; *N*-Methyl-*N*,2,4,6-tetranitroaniline; *N*-Methyl-*N*-picrylnitramine; *N*-Picryl-*N*-methylnitramine; NSC 2166; Nitramine; Nitramine (indicator); Picrylmethylnitramine; Picrylnitromethylamine; Tetralit; Tetralite; Tetril; Tetryl

**CA Index Name** Benzenamine, *N*-methyl-*N*,2,4,6-tetranitro-

**CAS Registry Number** 479-45-8

**Merck Index Number** 6573

### Chemical Structure



**Chemical/Dye Class** Nitro

**Molecular Formula** C<sub>7</sub>H<sub>5</sub>N<sub>5</sub>O<sub>8</sub>

**Molecular Weight** 287.14

**pH Range** 10.8–13.0

**Color Change at pH** Colorless (10.8) to red-brown (13.0)

**pKa** 12.66

**Physical Form** Yellow crystals

**Solubility** Insoluble in water; soluble in ethanol, ether, benzene, acetic acid

**Melting Point** 130–132°C

**Boiling Point (Calcd.)** 503.7 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–11</sup>

**Major Applications** Explosives,<sup>2–3,9–17</sup> paints,<sup>18</sup> food storage<sup>19</sup>

**Safety/Toxicity** Cytotoxicity,<sup>20</sup> marine toxicity,<sup>21</sup> mutagenicity,<sup>22,23</sup> genotoxicity<sup>24</sup>

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## NITRAZINE YELLOW

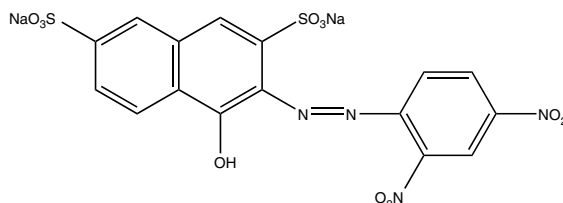
**Other Names** Nitrazine yellow; C.I. 14890; Delta Paper; Nitrazol Yellow

**CA Index Name** 2,7-Naphthalenedisulfonic acid, 3-[(2,4-dinitrophenyl)azo]-4-hydroxy-, disodium salt

**CAS Registry Number** 5423-07-4

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{16}H_8N_4O_{11}S_2Na_2$

**Molecular Weight** 542.37

**pH Range** 6.0–7.2

**Color Change at pH** Bright yellow (6.0) to bright blue (7.2)

**Physical Form** Red-brown powder

**Solubility** Soluble in water, acetic acid ethanol

**UV-Visible ( $\lambda_{max}$ )** 586 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Sensors,<sup>3–5</sup> display devices,<sup>6</sup> sol-gel matrix,<sup>7</sup> electrorheological materials,<sup>8</sup> diesel fuels/kerosines,<sup>9</sup> detergent,<sup>10</sup> fabric softener,<sup>11</sup> food storage,<sup>12</sup> method for identifying fresh & stale rice,<sup>13</sup> in dialysis solution,<sup>14</sup> screening of NAD-binding,<sup>15</sup> monitoring secreted body fluids,<sup>16</sup> locating lymph node,<sup>17</sup> diagnostic pads,<sup>18</sup> vaginal infection test method,<sup>19</sup> assay for esterolytic enzyme activity,<sup>20</sup> detecting pathogenic bacteria,<sup>21</sup> diagnosis of bacterial vaginosis,<sup>22</sup> detecting dysfunctional pregnancy,<sup>23</sup> drugs screening<sup>24,25</sup>

**Safety/Toxicity** No data available

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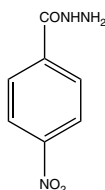
***p*-NITROBENZHYDRAZIDE**

**Other Names** Benzoic acid, *p*-nitro-, hydrazide; (*p*-Nitrobenzoyl)hydrazine; 4-Nitrobenzenecarboxylic acid hydrazide; 4-Nitrobenzhydrazide; 4-Nitrobenzohydrazide; 4-Nitrobenzoic acid hydrazide; 4-Nitrobenzoic hydrazide; 4-Nitrobenzoyl hydrazide; 4-Nitrobenzoylhydrazine; INHd 18; NSC 9804; *p*-Nitrobenzhydrazide; *p*-Nitrobenzohydrazide; *p*-Nitrobenzoic acid hydrazide; *p*-Nitrobenzoic hydrazide; *p*-Nitrobenzoyl hydrazide

**CA Index Name** Benzoic acid, 4-nitro-, hydrazide

**CAS Registry Number** 636-97-5

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Miscellaneous, Nitro, Hydrazide

**Molecular Formula** C<sub>7</sub>H<sub>7</sub>N<sub>3</sub>O<sub>3</sub>

**Molecular Weight** 181.15

**pH Range** 8.2–9.5

**Color Change at pH** Colorless (8.2) to yellow (9.5)

**pKa** 2.77, 11.17

**Physical Form** Yellow crystals

**Solubility** Insoluble in water; soluble in ethanol, methanol

**UV-Visible** (λ<sub>max</sub>) 267 nm

**Melting Point** 218°C (decompose)

**Synthesis** Synthetic methods<sup>1–9</sup>

**Major Applications** corrosion inhibitor,<sup>10,11</sup> disinfectant,<sup>1</sup> cosmetics,<sup>2</sup> paints<sup>3</sup> toothpaste,<sup>4</sup> mouthwash,<sup>4</sup> antifungal agent,<sup>12</sup> inhibit fibrosis,<sup>13</sup> antituberculosis agent<sup>14</sup>

**Safety/Toxicity** Toxicity,<sup>15</sup> teratogenicity,<sup>16</sup> acute oral toxicity<sup>17</sup>

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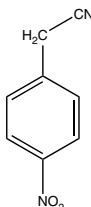
***p*-NITROBENZYL CYANIDE**

**Other Names** Acetonitrile, (*p*-nitrophenyl)-; (*p*-Nitrophenyl)acetonitrile; 4-Nitrobenzeneacetonitrile; 4-Nitrobenzyl cyanide; 4-Nitrophenylacetonitrile; NSC 5396; *p*-Nitro- $\alpha$ -tolunitrile; *p*-Nitrobenzeneacetonitrile; *p*-Nitrobenzyl cyanide

**CA Index Name** Benzeneacetonitrile, 4-nitro-

**CAS Registry Number** 555-21-5

**Merck Index Number** 6591

**Chemical Structure**

**Chemical/Dye Class** Miscellaneous, Nitro

**Molecular Formula** C<sub>8</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>

**Molecular Weight** 162.15

**pH Range** 11.4–12.9

**Color Change at pH** Yellow (11.4) to Orange-red (12.9)

**Physical Form** Yellow powder

**Solubility** Insoluble in water, soluble in ethanol, ether

**Melting Point** 117°C

**Boiling Point (Calcd.)** 336.3  $\pm$  17.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–18</sup>

**Major Applications** Recording materials,<sup>19,20</sup> photography,<sup>21,22</sup> forge-proof security paper,<sup>23</sup>

**Safety/Toxicity** toxicology,<sup>24</sup> acute toxicity,<sup>25</sup> oral toxicity<sup>26</sup>

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## 4-NITROCATECHOL

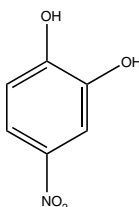
**Other Names** Pyrocatechol, 4-nitro-; 1,2-Dihydroxy-4-nitrobenzene; 3,4-Dihydroxy-1-nitrobenzene; 3,4-Dihydroxynitrobenzene; 4-Nitro-1,2-benzenediol; 4-Nitro-1,2-dihydroxybenzene; 4-Nitrobenzocatechin; 4-Nitrocatechol; 4-Nitropyrocatechol; NSC 80651; *p*-Nitrocatechol

**CA Index Name** 1,2-Benzenediol, 4-nitro-

**CAS Registry Number** 3316-09-4

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Nitro

**Molecular Formula**  $C_6H_5NO_4$

**Molecular Weight** 155.11

**pH Range** 3.9–6.3

**Color Change at pH** Straw (3.9) to lemon yellow (6.3)

**pKa** 6.84

**Physical Form** Light yellow crystals

**Solubility** Very slightly soluble in water; soluble in ethanol

**UV-Visible ( $\lambda_{max}$ )** 385 nm, 510 nm

**Melting Point** 174–176°C

**Boiling Point (Calcd.)**  $358.2 \pm 32.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–12</sup>

**Major Applications** Semiconductors,<sup>13</sup> magnetic recording materials,<sup>14</sup> nonlinear optical materials,<sup>15</sup> photography,<sup>16</sup> determination of lysosomal enzyme disorders,<sup>17</sup> antimicrobial agent,<sup>18</sup> anti-cancer agent<sup>19</sup>

**Safety/Toxicity** Chemistry-toxicity relationship,<sup>20</sup> ecotoxicity,<sup>21</sup> toxicity,<sup>22</sup> cytotoxicity,<sup>23</sup> phytotoxicity<sup>24</sup>

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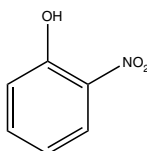
**o-NITROPHENOL**

**Other Names** Phenol, *o*-nitro-; 2-Hydroxynitrobenzene; 2-Nitrophenol; NSC 1552; *o*-Hydroxynitrobenzene; *o*-Nitrophenol

**CA Index Name** Phenol, 2-nitro-

**CAS Registry Number** 88-75-5

**Merck Index Number** 6620

**Chemical Structure**

**Chemical/Dye Class** Nitro

**Molecular Formula** C<sub>6</sub>H<sub>5</sub>NO<sub>3</sub>

**Molecular Weight** 139.11

**pH Range** 5.0–7.0

**Color Change at pH** Colorless (5.0) to yellow (7.0)

**pKa** 7.14, 7.22

**Physical Form** Light yellow crystals

**Solubility** Sparingly soluble in water; soluble in ethanol, ether, benzene

**Melting Point** 44–45°C

**Boiling Point** 214–216°C

**Synthesis** Synthetic methods<sup>1–12</sup>

**Major Applications** High voltage capacitors,<sup>13,14</sup> inks,<sup>15</sup> energetic materials,<sup>16</sup> corrosion inhibitors,<sup>17,18</sup> fertilizer,<sup>19</sup> food storage,<sup>20</sup> enzyme assays,<sup>21</sup> detecting microorganisms,<sup>22</sup> immunotherapy,<sup>23</sup> drugs<sup>24</sup>

**Safety/Toxicity** Chemical toxicity,<sup>25,26</sup> ecotoxicity,<sup>27</sup> acute toxicity,<sup>28</sup> toxicology,<sup>29</sup> mutagenicity,<sup>30</sup> immunotoxicology,<sup>31</sup> genotoxicity,<sup>32</sup> hepatotoxicity,<sup>33</sup> cytotoxicity,<sup>33</sup> phytotoxicity<sup>34</sup>

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***m*-NITROPHENOL**

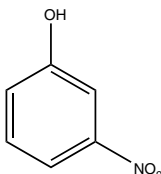
**Other Names** Phenol, *m*-nitro-; 1-Hydroxy-3-nitrobenzene; 3-Hydroxynitrobenzene; 3-Nitrophenol; NSC 1551; *m*-Hydroxynitrobenzene; *m*-Nitrophenol

**CA Index Name** Phenol, 3-nitro-

**CAS Registry Number** 554-84-7

**Merck Index Number** 6619

**Chemical Structure**



**Chemical/Dye Class** Nitro

**Molecular Formula** C<sub>6</sub>H<sub>5</sub>NO<sub>3</sub>

**Molecular Weight** 139.11

**pH Range** 6.8–8.6

**Color Change at pH** Colorless (6.8) to yellow (8.6)

**pKa** 8.34, 8.30, 8.33

**Physical Form** Yellow to orange-brown crystals

**Solubility** Sparingly soluble in water; soluble in ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 570 nm

**Melting Point** 97–98°C

**Boiling Point** 277°C

**Synthesis** Synthetic methods<sup>1–11</sup>

**Major Applications** Display device,<sup>12</sup> semiconductor device,<sup>13</sup> sensors,<sup>14</sup> high voltage capacitors,<sup>15</sup> energetic materials,<sup>16</sup> electrolyte batteries,<sup>17</sup> inks,<sup>18</sup> correction fluid,<sup>19</sup> detergent,<sup>20</sup> leak detection method,<sup>21</sup> lubricants,<sup>22</sup> insecticide,<sup>23</sup> food storage,<sup>24</sup> inhibition of amyloidoses,<sup>25</sup> detect bacterial infection,<sup>26</sup> drugs,<sup>27</sup> material for evaluating dental caries activity<sup>28</sup>

**Safety/Toxicity** Chemical toxicity,<sup>29,30</sup> ecotoxicity,<sup>31</sup> acute toxicity,<sup>32</sup> toxicology,<sup>33</sup> mutagenicity,<sup>34</sup> immunotoxicology,<sup>35</sup> genotoxicity,<sup>36</sup> hepatotoxicity,<sup>37</sup> cytotoxicity,<sup>37</sup> phytotoxicity<sup>38</sup>

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37. Shoji, R.; Sakoda, A.; Sakai, Y.; Utsumi, H.; Suzuki, M. A new assay for evaluating hepatotoxicity and cytotoxicity using LDL-uptake activity of liver cells. *J. Health Sci.* **2000**, *46*, 493–502.
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## *p*-NITROPHENOL

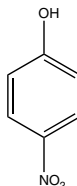
**OtherNames** Phenol,*p*-nitro-; 1-Hydroxy-4-nitrobenzene; 4-Hydroxy-1-nitrobenzene; 4-Hydroxynitrobenzene; 4-Nitrophenol; NSC 1317; Niphen; *p*-Hydroxynitrobenzene; *p*-Nitrophenol

**CA Index Name** Phenol, 4-nitro-

**CAS Registry Number** 100-02-7

**Merck Index Number** 6621

**Chemical Structure**



**Chemical/Dye Class** Nitro

**Molecular Formula** C<sub>6</sub>H<sub>5</sub>NO<sub>3</sub>

**Molecular Weight** 139.11

**pH Range** 5.6–7.6

**Color Change at pH** Colorless (5.6) to yellow (7.6)

**pKa** 7.15

**Physical Form** Yellow crystals

**Solubility** Sparingly soluble in water; soluble in ethanol, ether, chloroform

**UV-Visible** ( $\lambda_{\text{max}}$ ) 320 nm, 405 nm

**Melting Point** 113–114°C

**Boiling Point** 279°C

**Synthesis** Synthetic methods<sup>1–15</sup>

**Major Applications** Display device,<sup>16</sup> solar cells,<sup>17</sup> nanoparticles,<sup>18</sup> electrolytic capacitors,<sup>19,20</sup> lithographic printing plate,<sup>21</sup> leak detection method,<sup>22</sup> falsification-proof security paper,<sup>23</sup> correction fluid,<sup>24</sup> detergent,<sup>25</sup> fertilizer,<sup>26</sup> identifying fresh and stale rice,<sup>27</sup> diapers,<sup>28</sup> detecting lactic acid bacteria,<sup>29</sup> drug delivery,<sup>30</sup> evaluating dental caries activity<sup>31</sup>

**Safety/Toxicity** Aquatic toxicity,<sup>32</sup> chemical toxicity,<sup>33</sup> cytotoxicity,<sup>34</sup> ecotoxicity,<sup>35</sup> genotoxicity,<sup>36</sup> hepatotoxicity,<sup>37</sup> immunotoxicity,<sup>37</sup> mutagenicity,<sup>38</sup> neurotoxicity<sup>39</sup>

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# O

## ORANGE II

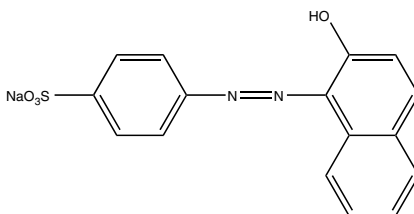
**Other Names** Acid Orange; Acid Orange A; C.I. Acid Orange 7, monosodium salt; Benzenesulfonic acid, *p*-(2-hydroxy-1-naphthylazo)-, sodium salt;  $\beta$ -Naphthol Orange;  $\beta$ -Naphthyl orange; 11550 Orange; 2-Naphthol Orange II; AO 7; Acid Leather Orange PRW; Acid Leather Orange extra; Acid Orange 7; Acid Orange II; Acilan Orange II; Airedale Orange II; Amacid Orange Y; Amacid Orange Y Conc; Atul Acid Orange II; Basacid Orange 280; Basacid Orange 282; Betanaphthol orange; Brasilan Orange A; Bucacid Orange A; C Ext. Orange 8; C.I. 15510; C.I. Acid Orange 7; Calcocid Orange Y; Certiquel Orange II; Colacid Orange; Curol Orange; D and C Orange No. 4; D&C Orange #4; D&C Orange No. 4; Diacid Orange II; Duasyn Acid Orange P; Egacid Orange II; Erio Orange II; Everacid Orange II; Fenazo Orange; Hidacid Orange II; Hispacid Orange AF; Japan Orange 205; Japan Orange No. 205; Java Orange II; Keyacid Orange II; Kiton Orange II; Kromon Lake Orange Toner; Lake Orange A; Lake Orange II YS; Leather Orange Extra; Lurazol Orange E; Lurazol Orange EBR; Lutetia Orange 3JR; Mandarin G; Naphthalene Lake Orange G; Naphthalene Orange G; Naphthol Orange; Naphtocard Orange II; Neklacid Orange II; No. 177 Orange Lake; Nubilon Orange R; Orange 2; Orange 2 sodium salt; Orange Extra N; Orange Extra P; Orange II; Orange II Special For Lacquer; Orange II for Lakes; Orange IIC; Orange IIP; Orange IIS; Orange IISM; Orange No. 205; Orange Toner GRT; Orange Y; Orange YA; Orange YZ; Peer-acid Orange II; Persian Orange; Persian Orange Lake; Persian Orange X; Pure Orange II S; Rifa Acid Orange II; Rybacel Orange A; Sanyo Gum Orange A; Sodium 4-(2-hydroxy-1-naphthylazo)benzenesulfonate; Solar Orange; Special Orange GR; Special Orange H; Symuler Orange Lake 43; Symulon Acid Orange II; Takaoka Acid Orange II; Tangarine Lake X 917; Tertracid Orange II; Tropaeolin OOO; Tropaeolin OOO 2; Tropeolin OOO; Vondacid Orange II; Wool Orange A; *p*-(2-Hydroxy-1-naphthylazo)benzenesulfonic acid sodium salt

**CA Index Name** Benzenesulfonic acid, 4-[(2-hydroxy-1-naphthalenyl)azo]-, monosodium salt

**CAS Registry Number** 633-96-5

**Merck Index Number** 6858

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{16}H_{11}N_2O_4SNa$

**Molecular Weight** 350.33

**pH Range** 7.4–8.6;

10.2–11.8

**Color Change at pH** Amber (7.4) to orange (8.6)

Orange (10.2) to red (11.8)

**pKa** 8.26, 11.4

**Physical Form** Orange-brown powder

**Solubility** Very soluble in water; very slightly soluble in ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 483 nm

**Melting Point** >300°C

**Synthesis** Synthetic methods<sup>1–6</sup>

**Major Applications** Organic light emitting diodes (OLEDs),<sup>7</sup> nanoparticles,<sup>8</sup> inks,<sup>9</sup> wood preservatives,<sup>10</sup> textiles,<sup>11</sup> hair dyes,<sup>12,13</sup> cosmetics,<sup>14,15</sup> wound dressing materials,<sup>16</sup> biofuel cells<sup>17</sup>

**Safety/Toxicity** Acute toxicity,<sup>18</sup> carcinogenicity,<sup>19</sup> genotoxicity,<sup>20</sup> toxicity to fish,<sup>21</sup> mutagenicity<sup>22,23</sup>

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## ORANGE III

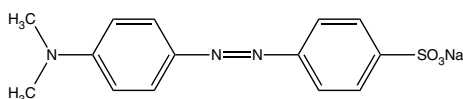
**Other Names** Benzenesulfonic acid, *p*-[[*p*-(dimethylamino)phenyl]azo]-, sodium salt; Orange III; 4-Dimethylaminoazobenzene-4'-sulfonic acid sodium salt; C.I. 13025; C.I. Acid Orange 52; Diazoben; Eniamethyl Orange; Gold orange; Helianthine; Helianthine B; KCA Methyl Orange; Methyl Orange B; Methyl orange; Orange 3; Sodium 4'-(dimethylamino)azobenzene-4-sulfonate; Sodium 4-(dimethylamino)azobenzene-4'-sulfonate; Sodium 4-[4-(dimethylamino)-phenylazo]-benzenesulfonate; Sodium *p*-[*p*-(dimethylamino)-phenylazo]-benzenesulfonate; Sodium *p*-dimethylaminoazobenzenesulfonate; Tropaeolin D

**CA Index Name** Benzenesulfonic acid, 4-[[4-(dimethylamino)phenyl]azo]-, sodium salt

**CAS Registry Number** 547-58-0

**Merck Index Number** 6105

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>14</sub>H<sub>14</sub>N<sub>3</sub>O<sub>3</sub>Na

**Molecular Weight** 327.34

**pH Range** 3.0–4.4

**Color Change at pH** Red (3.0) to yellow (4.4)

**pKa** 3.76, 3.40

**Physical Form** Orange powder

**Solubility** Slightly soluble in water, more soluble in hot water; practically insoluble in ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 507 nm, 522 nm, 464 nm

**Melting Point** >300°C

**Synthesis** Synthetic methods<sup>1–9</sup>

**Major Applications** Liquid crystals,<sup>10</sup> thin films,<sup>11</sup> sensors,<sup>12</sup> sol-gel matrix,<sup>13</sup> waveguides,<sup>14</sup> host-guest chemistry,<sup>15</sup> display device,<sup>16</sup> corrosion inhibitor,<sup>17</sup> glass coatings,<sup>18</sup> paints,<sup>19</sup> wound dressing materials,<sup>20</sup> pharmaceuticals,<sup>21</sup> dental materials,<sup>22</sup> measuring nucleic acid<sup>23</sup>

**Safety/Toxicity** Carcinogenicity,<sup>24</sup> genotoxicity,<sup>25</sup> mutagenicity<sup>26</sup>

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## ORANGE IV

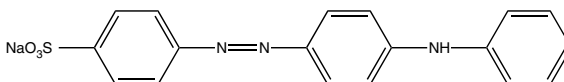
**Other Names** Benzenesulfonic acid, *p*-(*p*-anilinophenylazo)-, sodium salt; C.I. Acid Orange 5; C.I. Acid Orange 5, monosodium salt; Acid Orange 5; Acid Orange IV; Acid Yellow D; Aniline Yellow; C.I. 13080; Diphenylamine Orange; Hispacid Orange IV; Orange GS; Orange IV; Orange N; Solar Orange IV; Tertracid Orange IV; Tropaeolin OO; Tropeolin OO

**CA Index Name** Benzenesulfonic acid, 4-[[4-(phenylamino)phenyl]azo]-, monosodium salt

**CAS Registry Number** 554-73-4

**Merck Index Number** 9776

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>18</sub>H<sub>14</sub>N<sub>3</sub>O<sub>3</sub>SNa

**Molecular Weight** 375.38

**pH Range** 1.4–2.6

**Color Change at pH** Red (1.4) to yellow (2.6)

**pKa** 2.0

**Physical Form** Orange-yellow powder

**Solubility** Soluble in water, ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 527 nm, 443 nm

**Melting Point** >300°C

**Synthesis** Synthetic methods<sup>1–4</sup>

**Major Applications** Sensors,<sup>5</sup> lithographic plates,<sup>6</sup> optical recording media,<sup>7</sup> photoreceptor,<sup>8</sup> inks,<sup>9</sup> indication system for product exceeding threshold temperature,<sup>10</sup> lubricants,<sup>11</sup> textiles,<sup>12</sup> food storage,<sup>13</sup> determination of amiodarone,<sup>14</sup> astemizole,<sup>15</sup> bromhexine,<sup>16</sup> clomipramine,<sup>17</sup> deuterforin,<sup>18</sup> domperidone,<sup>19</sup> fluoroquinolone,<sup>20</sup> roxithromycin,<sup>21</sup> terfenadine,<sup>22</sup> thiabendazole,<sup>23</sup> antihistamines<sup>24</sup>

**Safety/Toxicity** Biodegradation and toxicity<sup>25</sup>

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**OREGON GREEN 488 CARBOXYLIC ACID**

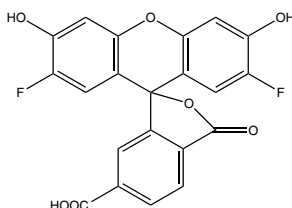
**Other Names** Oregon Green 488 carboxylic acid

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 2',7'-difluoro-3',6'-dihydroxy-3-oxo-

**CAS Registry Number** 195136-52-8

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>21</sub>H<sub>10</sub>F<sub>2</sub>O<sub>7</sub>

**Molecular Weight** 412.30

**pH Range** 4.2–5.7

**Color Change at pH** Weak green fluorescence (4.2) to strong green fluorescence (5.7)

**pKa** 4.7

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in *N,N*-dimethylformamide

**UV-Visible** ( $\lambda_{\text{max}}$ ) 478 nm, 492 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 693.9 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Sensors,<sup>4</sup> methods of determining human blood-relationship,<sup>5</sup> method for purifying actin in plant cells,<sup>6</sup> phagosomal pH determination<sup>7</sup>

**Safety/Toxicity** No data available

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**OREGON GREEN 514 CARBOXYLIC ACID**

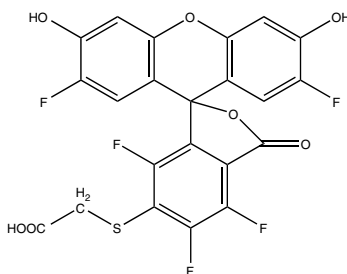
**Other Names** Oregon Green 514 carboxylic acid 6-isomer

**CA Index Name** Acetic acid, [(2',4,5,7,7'-pentafluoro-3',6'-dihydroxy-3-oxospiro-[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)thio]-

**CAS Registry Number** 198139-49-0

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>22</sub>H<sub>9</sub>F<sub>5</sub>O<sub>7</sub>S

**Molecular Weight** 512.36

**pH Range** 4.2–5.7

**Color Change at pH** Weak green fluorescence (4.2) to strong green fluorescence (5.7)

**pKa** 4.7

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in *N,N*-dimethylformamide

**UV-Visible** ( $\lambda_{\text{max}}$ ) 489 nm, 506 nm

**Melting Point** >250°C

**Boiling Point (calcd.)** 703.2 ± 60.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Method for measuring stress biomarkers in body fluids,<sup>4</sup> method for diagnostic & therapeutic transport,<sup>5</sup> monitoring protein conformation,<sup>6</sup> detecting bacteria,<sup>7</sup> delivering nucleic acids & proteins across skin,<sup>8</sup> method for determining size of polynucleotides,<sup>9</sup> probing the diffusion in ultrathin films,<sup>10</sup> genotyping of nucleic acid polymorphisms,<sup>11</sup> molecular clasps,<sup>12</sup> measuring protein–protein & protein–nucleic acid interactions,<sup>13</sup> analysis of the protein distribution,<sup>14</sup> detecting gene expression,<sup>15</sup> as geothermal tracers,<sup>16</sup> determination of biomolecules,<sup>17</sup> pH sensors<sup>18</sup>

**Safety/Toxicity** No data available

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**OREGON GREEN 488 CARBOXYLIC ACID DIACETATE**

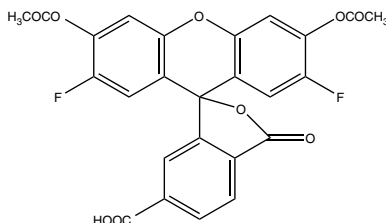
**Other Names** Oregon Green 488 carboxylic acid diacetate

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 3',6'-bis(acetyloxy)-2',7'-difluoro-3-oxo-

**CAS Registry Number** 195136-74-4

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Xanthene

**Molecular Formula** C<sub>25</sub>H<sub>14</sub>F<sub>2</sub>O<sub>9</sub>

**Molecular Weight** 496.37

**pH Range** 4.2–5.7

**Color Change at pH** Weak green fluorescence (4.2) to strong green fluorescence (5.7)

**pKa** 4.65

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in *N,N*-dimethyl formamide, dimethyl sulfoxide

**UV-Visible ( $\lambda_{\text{max}}$ )** <300 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 691.5 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Electrical lysis of cells,<sup>3</sup> detecting anion transport mechanism at the tonoplast,<sup>4</sup> as tracers and for preparing conjugates of organic & inorganic substances<sup>1</sup>

**Safety/Toxicity** No data available

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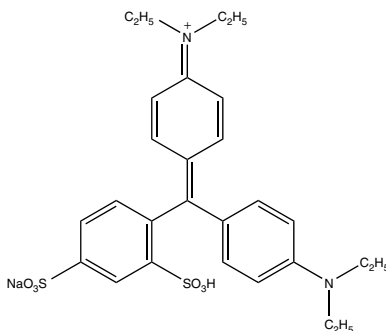
## PATENT BLUE V

**Other Names** C.I. Acid Blue 1, sodium salt; Ethanaminium, *N*-[4-[[4- (diethylamino)phenyl](2, 4-disulphophenyl)methylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-, hydroxide, inner salt, sodium salt; Xylene Blue VS; [4-[ $\alpha$ -[*p*-(Diethylamino)phenyl]-2,4-isulphobenzylidene]-2,5-cyclohexadien-1-ylidene]-diethylammonium hydroxide, inner salt, sodium salt; 1085 Blue; Acid Blue 1; Acid Blue V; Acid Bright Azure Z; Acid Brilliant Blue Z; Acid Brilliant Sky Blue Z; Acid Leather Blue V; Acid Turquoise Blue V; Aizen Brilliant Acid Pure Blue VH; Alphazurine 2G; Amacid Blue V; Bleu Patente V; Blue URS; Blue VRS; Brilliant Acid Blue A Export; Brilliant Acid Blue V Extra; Brilliant Acid Blue VS; Brilliant Blue GS; Bucacid Patent Blue VF; C.I. 42045; C.I. Acid Blue 1; C.I. Food Blue 3; Carmine Blue VF; Disulfine blue VN; Disulphine Blue VN; Disulphine Blue VN 150; Disulphine VN; Duasyn Acid Blue V 02; Edicol Supra Blue VR; Erioglaucine supra; Fenazo Blue XF; Hexacol Blue VRS; Hidacid Blue V; Kiton Pure Blue V; Kiton Pure Blue V.FQ; Leather Blue G; Merantine Blue VF; Orient Water Blue 106; Patent Blue; Patent Blue V; Patent Blue VF; Patent Blue VF Special; Patent Blue VF-CF; Patent Pure Blue VX; Patent blue VS; Patent blue violet; Pontacyl Brilliant Blue V; Sodium Blue VRS; Sodium Patent Blue V; Sulfan blue; Sulphan Blue; Sumitomo Patent Pure Blue VX; Tertracid Carmine Blue V

**CA Index Name** Ethanaminium, *N*-[4-[[4-(diethylamino)phenyl](2,4- disulphophenyl)methylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-, inner salt, sodium salt

**CAS Registry Number** 129-17-9

**Merck Index Number** 8987

**Chemical Structure**

**Chemical/Dye Class** Triphenylmethane

**Molecular Formula**  $C_{27}H_{31}N_2O_6S_2Na$

**Molecular Weight** 566.68

**pH Range** 0.8–3.0

**Color Change at pH** Yellow-orange (0.8) to deep blue (3.0)

**Physical Form** Dark blue powder

**Solubility** Soluble in water; partly soluble in ethanol; insoluble in xylene

**UV-Visible** ( $\lambda_{max}$ ) 635 nm, 410 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1–3</sup>



**Major Applications** Liquid crystal displays,<sup>4</sup> color filters,<sup>5,6</sup> electrorheological materials,<sup>7</sup> photographic materials,<sup>8</sup> optical filters,<sup>9</sup> inks,<sup>10</sup> highlighters,<sup>11</sup> dyeing paper,<sup>12</sup> wood dyeing,<sup>13</sup> textiles,<sup>14</sup> detergents,<sup>15</sup> hair dyes,<sup>16</sup> cosmetics,<sup>17</sup> lymph node identification,<sup>18</sup> antiparasitic agent,<sup>19</sup> nanocomposite particles for biomedical applications<sup>20</sup>

**Safety/Toxicity** Acute toxicity,<sup>21</sup> genotoxicity,<sup>22</sup> mutagenicity,<sup>23,24</sup> allergic reaction,<sup>25</sup> adverse reaction<sup>26</sup>

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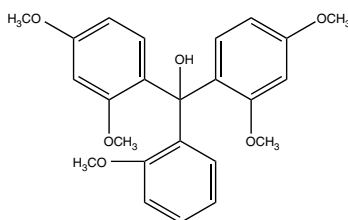
## PENTAMETHOXY RED

**Other Names** Methanol, *bis*(2,4-dimethoxyphenyl)(*o*-methoxyphenyl)-; 2,2',2'',4,4'-Pentamethoxytriphenylcarbinol; Pentamethoxy Red

**CA Index Name** Benzenemethanol,  $\alpha$ -(2,4-dimethoxyphenyl)-2,4-dimethoxy- $\alpha$ -(2-methoxyphenyl)-

**CAS Registry Number** 1755-51-7

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Triphenylmethane

**Molecular Formula** C<sub>24</sub>H<sub>26</sub>O<sub>6</sub>

**Molecular Weight** 410.46

**pH Range** 1.2–3.2

**Color Change at pH** Reddish-violet (1.2) to colorless (3.2)

**pKa** 1.86

**Physical Form** White crystals

**Solubility** Insoluble in water; soluble in ethanol

**Melting Point** 146–148°C

**Boiling Point (Calcd.)** 600.3 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Image producing materials,<sup>6–9</sup> recording materials,<sup>10–12</sup> resist composition,<sup>13</sup> xerographic copier materials,<sup>14</sup> inks,<sup>15</sup> cleaners,<sup>16</sup> cosmetics,<sup>16</sup> dental adhesives,<sup>17</sup>

**Safety/Toxicity** No data available

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## PHENOLBENZEIN

### P

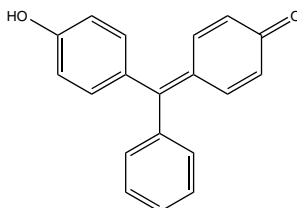
**Other Names** 2,5-Cyclohexadien-1-one, 4-(*p*-hydroxy- $\alpha$ -phenylbenzylidene)-; Benzaurin; NSC 55861; Phenolbenzein; Rosolic acid

**CA Index Name** 2,5-Cyclohexadien-1-one, 4-[(4-hydroxyphenyl)phenylmethylene]-

**CAS Registry Number** 569-60-8

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Benzein

**Molecular Formula** C<sub>19</sub>H<sub>14</sub>O<sub>2</sub>

**Molecular Weight** 274.31

**pH Range** 6.0–7.6

**Color Change at pH** Yellow (6.0) to red (7.6)

**pKa** 9.28

**Physical Form** Orange-red crystals

**Solubility** Insoluble in water; soluble in ethanol

**Melting Point** >250°C

**Boiling Point (Calcd.)** 497.0 ± 45.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Indicator<sup>6</sup>

**Safety/Toxicity** No data available

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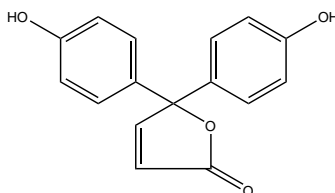
**PHENOLMALEIN**

**Other Names** 2(5H)-Furanone, 5,5-bis(*p*-hydroxyphenyl)-; Crotonic acid, 4- hydroxy-4,4-bis(*p*-hydroxyphenyl)-,  $\gamma$ -lactone; Phenolmalein

**CA Index Name** 2(5H)-Furanone, 5,5-bis(4-hydroxyphenyl)-

**CAS Registry Number** 1224-25-5

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Miscellaneous

**Molecular Formula** C<sub>16</sub>H<sub>12</sub>O<sub>4</sub>

**Molecular Weight** 268.26

**pH Range** 5.5–7.2

**Color Change at pH** Yellow (5.5) to red (7.2)

**pKa** 6.04

**Physical Form** Yellow crystals

**Solubility** Insoluble in water, soluble in ethanol, acetone

**Melting Point** 301°C

**Boiling Point (Calcd.)** 533.9  $\pm$  50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Bactericidal activity<sup>3</sup>

**Safety/Toxicity** No data available

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## P

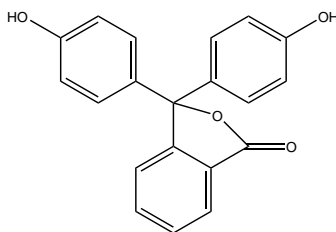
## PHENOLPHTHALEIN

**Other Names** Phenolphthalein; 3,3-Bis(4-hydroxyphenyl)-1(3H)-isobenzofuranone; 3,3-Bis(4-hydroxyphenyl)phthalide; 3,3-Bis(*p*-hydroxyphenyl)phthalide; Euchessina; Koprol; Laxogen; Lilo; NSC 10464; NSC 215214; Phthalimetten; Phthalin; Purga; Purgen; Purgophen; Spulmakolax; Trilax

**CA Index Name** 1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxyphenyl)-

**CAS Registry Number** 77-09-8

**Merck Index Number** 7243

**Chemical Structure**

**Chemical/Dye Class** Phthalein

**Molecular Formula** C<sub>20</sub>H<sub>14</sub>O<sub>4</sub>

**Molecular Weight** 318.32

**pH Range** 8.0–10.0

**Color Change at pH** Colorless (8.0) to pink (10.0)

**pKa** 9.10, 9.40, 9.53, 9.70

**Physical Form** White powder

**Solubility** Almost insoluble in water; soluble in alcohol, ether

**UV-Visible** ( $\lambda_{\text{max}}$ ) 552 nm, 553 nm, 374 nm, 205 nm, 229 nm, 276 nm

**Melting Point** 258–262°C

**Boiling Point (Calcd.)** 557.8 ± 50.0°C; Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–16</sup>

**Major Applications** Display device,<sup>17</sup> sensors,<sup>18</sup> semiconductors,<sup>19</sup> fuel cells,<sup>20</sup> photoreceptors,<sup>21</sup> electronic packaging,<sup>22</sup> authentication system for secure documents,<sup>23</sup> inks,<sup>24,25</sup> correction fluid,<sup>26</sup> paints,<sup>27</sup> detection of defects in films,<sup>28</sup> floor coatings,<sup>29</sup> textiles,<sup>30</sup> corrosion testing,<sup>31</sup> explosive,<sup>32</sup> concrete,<sup>33</sup> toys,<sup>34</sup> detecting lipase activity of crop seeds,<sup>35</sup> soaps,<sup>36</sup> method for prevention of drug misuse,<sup>37</sup> cosmetics,<sup>38</sup> diapers,<sup>39</sup> detecting viable cells,<sup>40</sup> carbohydrates,<sup>41</sup> antimalarial,<sup>42</sup> antibacterial,<sup>43</sup> treating amyloid-associated diseases<sup>44</sup>

**Safety/Toxicity** Bacterial toxicity,<sup>45</sup> ovarian cancer risk,<sup>46</sup> carcinogenicity,<sup>47–53</sup> genotoxicity,<sup>53–56</sup> mutagenicity,<sup>57</sup> toxicokinetics,<sup>58</sup> chromosomal aberration<sup>59,60</sup>

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## P

## PHENOLPHTHALEIN, DISODIUM SALT

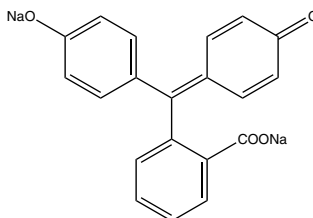
**Other Names** Phenolphthalein, disodium salt; Phenolphthalein sodium

**CA Index Name** 1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxyphenyl)-, disodium salt

**CAS Registry Number** 518-51-4

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Phthalein

**Molecular Formula**  $C_{20}H_{12}O_4Na_2$

**Molecular Weight** 362.29

**pH Range** 8.0–10.0

**Color Change at pH** Colorless (8.0) to pink (10.0)

**pKa** 9.1

**Physical Form** Dark red powder

**Solubility** Soluble in water, ethanol

**UV-Visible** ( $\lambda_{max}$ ) 553 nm

**Melting Point** >250°C

**Synthesis** Synthetic method<sup>1–3</sup>

**Major Applications** Inks,<sup>4</sup> fire-resistant polymers,<sup>5</sup> permanent hair straightener<sup>6</sup>

**Safety/Toxicity** No data available

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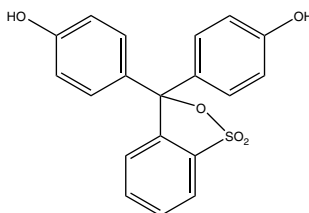
## PHENOL RED

**Other Names** Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)*bis*-, *S,S*-dioxide; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)*di*-, *S,S*-dioxide; 3H-2,1-Benzoxathiole, phenol deriv.;  $\alpha$ -Hydroxy- $\alpha,\alpha$ -*bis*(*p*-hydroxyphenyl)-*o*-toluenesulfonic acid  $\gamma$ -sultone; 3,3-*Bis*(*p*-hydroxyphenyl)-2,1,3H-benzoxathiole 1,1-dioxide; 3H-2,1-Benzoxathiole, 3,3-*bis*(4-hydroxyphenyl)-, 1,1-dioxide; Fenolipuna; NSC 10459; PSP; PSP (indicator); Phenol red; Phenolsulfonephthalein; Phenolsulfonphthalein; Phenolsulphonphthalein; Sulfonphthal; Sulphental; Sulphonthal; TF-R 2

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*-

**CAS Registry Number** 143-74-8

**Merck Index Number** 7247

**Chemical Structure**

**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>19</sub>H<sub>14</sub>O<sub>5</sub>S

**Molecular Weight** 354.38

**pH Range** 6.8–8.4

**Color Change at pH** Yellow (6.8) to red (8.4)

**pKa** 7.90

**Physical Form** Red crystals

**Solubility** Sparingly soluble in water; soluble in ethanol; almost insoluble in ether, chloroform

**UV-Visible** ( $\lambda_{\text{max}}$ ) 557 nm, 558 nm, 360 nm, 423 nm, 433 nm

**Melting Point** >300°C

**Boiling Point (Calcd.)** 562.8  $\pm$  50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1-6</sup>

**Major Applications** Display device,<sup>7</sup> sol-gel matrix,<sup>8</sup> photoreceptors,<sup>9</sup> fuel cells,<sup>10</sup> waveguides,<sup>11</sup> paints,<sup>12</sup> detergents,<sup>13</sup> cosmetics,<sup>14</sup> antiperspirant composition,<sup>15</sup> diapers,<sup>16</sup> screening bacteria,<sup>17</sup> detecting viable cells,<sup>18</sup> diagnosis of urogenital ureaplasmosis,<sup>19</sup> treatment of pathogen infections,<sup>20</sup> amyloid-associated diseases,<sup>21</sup> glaucoma,<sup>22</sup> pulmonary hypertension,<sup>22</sup> asthma,<sup>22</sup> chronic obstructive pulmonary disease,<sup>22</sup> erectile dysfunction,<sup>22</sup> Raynaud's syndrome,<sup>22</sup> heparin overdose,<sup>22</sup> vulvodysnia,<sup>22</sup> wound healing,<sup>22</sup> psychoactive drugs,<sup>23</sup> evaluating dental caries activity<sup>24</sup>

**Safety/Toxicity** Carcinogenicity,<sup>25</sup> environmental analysis,<sup>26</sup> dye-induced cholestasis,<sup>27</sup> mutagenicity,<sup>28</sup> Nephrotoxicity<sup>29,30</sup>

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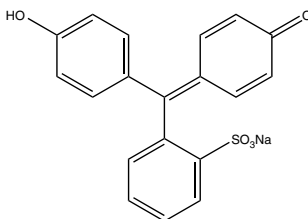
**PHENOL RED, SODIUM SALT**

**Other Names** Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)*bis*-, *S,S*-dioxide, monosodium salt; 3H-2,1-Benzoxathiole, phenol deriv.; Phenol red sodium; Phenol red, sodium salt; Phenolsulfonephthalein sodium

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*-, monosodium salt

**CAS Registry Number** 34487-61-1

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>19</sub>H<sub>13</sub>O<sub>5</sub>SNa

**Molecular Weight** 376.36

**pH Range** 6.8–8.4

**Color Change at pH** Yellow (6.8) to red (8.4)

**pKa** 7.69, 7.9, 1.3

**Physical Form** Shiny dark-red crystals

**Solubility** Soluble in water, ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 423 nm, 557 nm

**Melting Point** 285°C

**Synthesis** Synthetic method<sup>1–3</sup>

**Major Applications** Sensor,<sup>4</sup> optical device,<sup>5</sup> paints,<sup>6</sup> sterilization process,<sup>7</sup> fertilizer,<sup>8</sup> detecting viable cells,<sup>9</sup> gastrointestinal mucosa,<sup>10</sup> antibacterial agent,<sup>11</sup> drugs,<sup>12</sup> pharmacology<sup>13</sup>

**Safety/Toxicity** Toxic blocking activity<sup>13</sup>

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### 4-(PHENYLAZO)-DIPHENYLAMINE

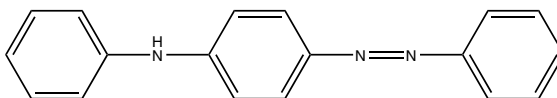
**Other Names** Diphenylamine, 4-(phenylazo)-; 4-(Phenylamino)azobenzene; 4- (Phenylazo)diphenylamine; 4-Anilinoazobenzene; 4- Phenazodiphenylamine; *N*-Phenyl-4-(phenylazo)aniline; *N*- Phenyl-4-(phenylazo)benzenamine; *N*-Phenyl-4-aminoazobenzene; NSC 74774

**CA Index Name** Benzenamine, *N*-phenyl-4-(phenylazo)-

**CAS Registry Number** 101-75-7

**Merck Index Number** Not listed

#### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>18</sub>H<sub>15</sub>N<sub>3</sub>

**Molecular Weight** 273.33

**pH Range** 1.2–2.5

**Color Change at pH** Red (1.2) to yellow (2.5)

**pKa** 0.42

**Physical Form** Orange powder

**Solubility** Insoluble in water; soluble in ethanol, methanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 411 nm, 272 nm

**Melting Point** 89–91°C

**Boiling Point (Calcd.)** 451.7 ± 28.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–12</sup>

**Major Applications** Display device,<sup>13</sup> nonlinear optical (NLO) material,<sup>14</sup> photoresists,<sup>15</sup> printing plates,<sup>16,17</sup> lithographic plates,<sup>18</sup> photosensitive materials,<sup>19</sup> photography,<sup>20</sup> markers<sup>21</sup>

**Safety/Toxicity** Oral toxicity<sup>22</sup>

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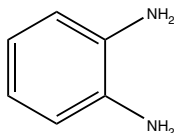
**o-PHENYLENEDIAMINE**

**Other Names** *o*-Phenylenediamine; 1,2-Diaminobenzene; 1,2-Phenylenediamine; 2-Aminoaniline; C.I. 76010; C.I. Oxidation Base 16; IK 3; IK 3 (amine); NSC 5354; Orthamine; *o*-Aminoaniline; *o*-Aminophenylamine; *o*-Benzenediamine; *o*-Diaminobenzene

**CA Index Name** 1,2-Benzenediamine

**CAS Registry Number** 95-54-5

**Merck Index Number** 7284

**Chemical Structure**

**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>

**Molecular Weight** 108.14

**pH Range** 3.1–4.4

**Color Change at pH** Green fluorescence (3.1) to nonfluorescence (4.4)

**pKa** 4.46

**Physical Form** Brown crystals

**Solubility** Slightly soluble in water; freely soluble in ethanol, ether, chloroform

**Melting Point** 103–104°C

**Boiling Point** 256–258°C

**Synthesis** Synthetic methods<sup>1–8</sup>

**Major Applications** Bottom antireflective coatings,<sup>9</sup> semiconductor devices,<sup>10</sup> hair dyes,<sup>11</sup> detecting antibody,<sup>12</sup> glucose,<sup>13</sup> streptomycin,<sup>14</sup> penicillin,<sup>15</sup> sulfonamide,<sup>16</sup> neuroglobin,<sup>17</sup> substrate for horse radish peroxidase<sup>18</sup>

**Safety/Toxicity** Acute toxicity,<sup>19</sup> aquatic toxicity,<sup>20</sup> carcinogenicity,<sup>21</sup> chemical toxicity,<sup>22</sup> hepatotoxicity,<sup>23</sup> cytotoxicity,<sup>23</sup> genotoxicity,<sup>24</sup> mutagenicity,<sup>25,26</sup> oral toxicity,<sup>27</sup> percutaneous toxicity,<sup>28</sup> phytotoxicity<sup>29</sup>

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## P

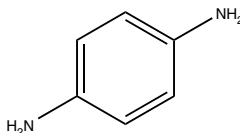
***p*-PHENYLENEDIAMINE**

**OtherNames** *p*-Phenylenediamine; 1,4-Diaminobenzene; 1,4-Diaminobenzol; 1,4-Phenylenediamine; 4-Aminoaniline; BASF Ursol D; Benzofur D; Black for Fur D; C.I. 76060; C.I. Developer 13; C.I. Oxidation Base 10; Developer PF; Durafur Black R; Fouramine D; Fournine 1; Fournine D; Fur Black 41867; Fur Brown 41866; Fur Yellow; Furro D; Futramine D; NSC 4777; Nako H; Orsin; PPD; Pelagol D; Pelagol DR; Pelagol Grey D; Peltol D; Renal PF; Rodol DJ; Tertral D; Ursol D; Zoba Black D; *p*-Aminoaniline; *p*-Benzenediamine; *p*-Diaminobenzene

**CA Index Name** 1,4-Benzenediamine

**CAS Registry Number** 106-50-3

**Merck Index Number** 7285

**Chemical Structure**

**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>

**Molecular Weight** 108.14

**pH Range** 3.1–4.4

**Color Change at pH** Nonfluorescence (3.1) to orange/yellow fluorescence (4.4)

**pKa** 4.17

**Physical Form** White to slightly red crystals, darkens on exposure to air

**Solubility** Slightly soluble in water; soluble in ethanol, ether, chloroform

**Melting Point** 145–147°C

**Boiling Point** 267°C

**Synthesis** Synthetic methods<sup>1–10</sup>

**Major Applications** Nanoparticles,<sup>11</sup> liquid crystal displays,<sup>12</sup> chemical mechanical polishing,<sup>13</sup> bottom antireflective coatings,<sup>14</sup> electrochromic materials,<sup>15</sup> inks,<sup>16</sup> rubber,<sup>17</sup> hair dyes,<sup>18</sup> cosmetics,<sup>19</sup> treatment of virus skin infection<sup>20</sup>

**Safety/Toxicity** Acute toxicity,<sup>21</sup> cytotoxicity,<sup>21</sup> carcinogenicity,<sup>22</sup> genotoxicity,<sup>23</sup> mutagenicity<sup>24</sup>

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## P

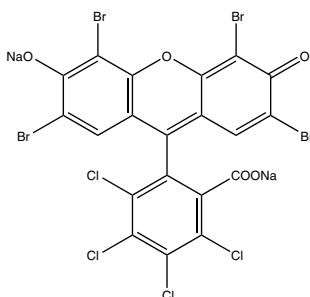
## PHLOXINE B

**Other Names** Fluorescein, 2',4',5',7'-tetrabromo-4,5,6,7-tetrachloro-, disodium salt; 11969 Red; 3427 Veri Pur Pink; Acid Red 92; Aizen Acid Phloxine PB; C.I. 45410; C.I. Acid Red 92; Cyanosin; Cyanosin (acid dye); Cyanosin B; Cyanosine; D and C Red No. 28; D&C Red 28; D&C Red No. 28; Daiwa Red 104WB; Daiwa Red 45; Disodium 9-(3',4',5',6'-tetrachloro-*o*-carboxyphenyl)-6-hydroxy-6-hydroxy-2,4,5,7-tetrabromo-3-isoxanthone; Eosin blue; Eosin bluish; Eosine blue; Eosine bluish; Food Red 104; Food Red No. 104; Japan Red 104; Japan Red 104-1; Orient Water Pink 2; Phloxine B; Phloxine P; Phyloxine B; Red 104; Red No. 104; Red No.104-1; Water Pink 2

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 2',4',5',7'-tetrabromo-4,5,6,7-tetrachloro-3',6'-dihydroxy-, disodium salt

**CAS Registry Number** 18472-87-2

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Xanthene, Fluorescent

**Molecular Formula** C<sub>20</sub>H<sub>2</sub>Br<sub>4</sub>Cl<sub>4</sub>O<sub>5</sub>Na<sub>2</sub>

**Molecular Weight** 829.66

**pH Range** 2.5–4.0

**Color Change at pH** Nonfluorescence (2.5) to yellowish-blue fluorescence (4.0)

**Physical Form** Brick-red powder

**Solubility** Soluble in water, ethylene glycol; slightly soluble in ethanol, methanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 548 nm, 510 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1–6</sup>

**Major Applications** Optical waveguides,<sup>7</sup> color filter,<sup>8</sup> lithographic printing plates,<sup>9</sup> display device,<sup>10</sup> inks,<sup>11–13</sup> highlighters,<sup>14</sup> textiles,<sup>15</sup> hair dyes,<sup>16</sup> cosmetics,<sup>17–19</sup> visualization of dental plaque,<sup>20</sup> treatment of infectitious diseases,<sup>21</sup> antitumor agents<sup>22</sup>

**Safety/Toxicity** Acute and chronic toxicity,<sup>23</sup> cytotoxicity,<sup>24</sup> estrogenicity,<sup>25</sup> eye irritation tests,<sup>26</sup> toxicity to insects,<sup>27</sup> mutagenicity,<sup>28</sup> oral toxicity,<sup>29</sup> phototoxicity,<sup>30</sup> teratogenicity,<sup>31</sup> topical toxicity<sup>32</sup>

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## PICRIC ACID

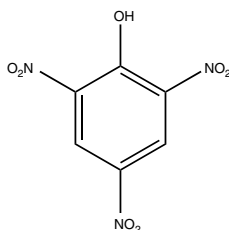
**Other Names** Picric acid; 1-Hydroxy-2,4,6-trinitrobenzene; 2,4,6-Trinitrophenol; C.I. 10305; Carbazotic acid; Melinite; NSC 36947; NSC 56147; Nitroxanthic acid; PA; Picral; Picronitric acid; Trinitrophenol

**CA Index Name** Phenol, 2,4,6-trinitro-

**CAS Registry Number** 88-89-1

**Merck Index Number** 7410

### Chemical Structure



**Chemical/Dye Class** Nitro

**Molecular Formula**  $C_6H_3N_3O_7$

**Molecular Weight** 229.10

**pH Range** 0.0–1.3

**Color Change at pH** Colorless (0.0) to yellow (1.3)

**pKa** 0.53

**Physical Form** Pale yellow glittering crystals

**Solubility** Soluble in water, ethanol, benzene, chloroform; insoluble in toluene

**UV-Visible ( $\lambda_{max}$ )** 354 nm

**Melting Point** 122–123°C

**Boiling Point (Calcd.)**  $303.6 \pm 42.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–8</sup>

**Major Applications** Explosives,<sup>9</sup> power circuits,<sup>10</sup> energetic materials,<sup>11</sup> liquefied gas fuels,<sup>12</sup> thin films,<sup>13</sup> power generation,<sup>14</sup> batteries,<sup>14,15</sup> fuel cells,<sup>16</sup> steel,<sup>17</sup> gold films,<sup>18</sup> nanopowder,<sup>19</sup> antifreeze fluid for automobiles,<sup>20</sup> polymerization inhibitors,<sup>21</sup> tattoo removal from skin,<sup>22</sup> antiinflammatory agent,<sup>23</sup> treatment of neoplasm<sup>24</sup>

**Safety/Toxicity** Acute toxicity,<sup>25,26</sup> algal toxicity,<sup>27,28</sup> toxicity to aquatic organisms,<sup>29</sup> toxicity to bacteria,<sup>30</sup> ecotoxicity,<sup>31</sup> environmental pollutants,<sup>32</sup> genotoxicity,<sup>33</sup> marine toxicity,<sup>34</sup> mutagenicity,<sup>35</sup> neurotoxicity<sup>36</sup>

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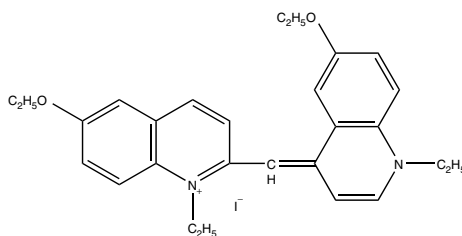
## PINACHROME

**Other Names** Quinolinium, 6-ethoxy-2-[(6-ethoxy-1-ethyl-4(1H)-quinolylidene)-methyl]-1-ethyl, iodide; Pinachrome; Pinachrome NK 914

**CA Index Name** Quinolinium, 6-ethoxy-2-[(6-ethoxy-1-ethyl-4(1H)-quinolinylidene)methyl]-1-ethyl-, iodide

**CAS Registry Number** 27593-93-7

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Quinoline

**Molecular Formula**  $C_{27}H_{31}N_2O_2I$

**Molecular Weight** 518

**pH Range** 5.6–8.0

**Color Change at pH** Colorless (5.6) to red-violet (8.0)

**pKa** 7.34

**Physical Form** Dark green powder

**Solubility** Soluble in water, ethanol, dilute hydrochloric acid (most commonly used)

**Melting Point**  $>250^{\circ}\text{C}$

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Inks,<sup>2</sup> dichromated gelatin,<sup>3</sup> photographic sensitizer<sup>4</sup>

**Safety/Toxicity** No data available

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**POIRRIER BLUE**

**Other Names** Poarie Blue C 4B  
**CA Index Name** Poirrier Blue C 4B  
**CAS Registry Number** 1400-96-0  
**Merck Index Number** Not listed  
**Chemical Structure** No structure diagram available  
**Chemical/Dye Class** Triphenylmethane  
**Molecular Formula** Unspecified  
**Molecular Weight** Not available  
**pH Range** 11.0–13.0  
**Color Change at pH** Blue (11.0) to violet-red (13.0)  
**Physical Form** Blue powder  
**Solubility** Soluble in water, ethanol  
**Melting Point** Not available  
**Synthesis** Synthetic method<sup>1</sup>  
**Major Applications** detecting degradation of concrete<sup>2</sup>  
**Safety/Toxicity** No data available

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## P

## PROPYL RED

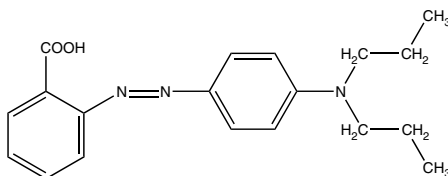
**Other Names** Benzoic acid, *o*-[[*p*-(dipropylamino)phenyl]azo]-; 2-[4-(Dipropylamino)phenylazo] benzoic acid; NSC 7803; Propyl red

**CA Index Name** Benzoic acid, 2-[[4-(dipropylamino)phenyl]azo]-

**CAS Registry Number** 2641-01-2

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>19</sub>H<sub>23</sub>N<sub>3</sub>O<sub>2</sub>

**Molecular Weight** 325.40

**pH Range** 4.6–6.6

**Color Change at pH** Red (4.6) to yellow (6.6)

**pKa** 5.48

**Physical Form** Yellow-orange solid

**Solubility** Insoluble in water; soluble in ethanol, methanol

**Melting Point** >250°C

**Boiling Point (Calcd.)** 515.8 ± 35.0°C Pressure: 760 Torr

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Electrophoresis display device,<sup>2</sup> image contrast-enhancing layer,<sup>3</sup> photography,<sup>4</sup> Photoelectrographic imaging,<sup>5</sup> inks,<sup>6</sup> paints,<sup>6</sup> toys<sup>6</sup>

**Safety/Toxicity** No data available

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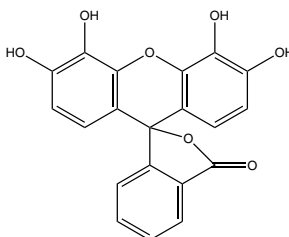
## PYROGALLOLPHTHALEIN

**Other Names** Gallein; Alizarine violet; C.I. 45445; C.I. Mordant Violet 25; Mordant Violet 25; NSC 56445; NSC 622478; NSC 8668; Pyrogallolphthalein

**CA Index Name** Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',4',5',6'-tetrahydroxy-

**CAS Registry Number** 2103-64-2

**Merck Index Number** 4344

**Chemical Structure**

**Chemical/Dye Class** Miscellaneous, Xanthene

**Molecular Formula**  $C_{20}H_{12}O_7$

**Molecular Weight** 364.31

**pH Range** 3.8–6.6;

10.6–13.0

**Color Change at pH** Yellow (3.8) to rose-red (6.6)

Pink (10.6) to violet (13.0)

**pKa** 5.99

**Physical Form** Brownish-red powder

**Solubility** Almost insoluble in water, benzene, chloroform; soluble in ethanol, acetone

**Melting Point**  $>300^{\circ}\text{C}$

**Boiling Point (Calcd.)**  $687.4 \pm 55.0^{\circ}\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–7</sup>

**Major Applications** Organic light emitting devices (OLED),<sup>8</sup> semiconductors,<sup>9,10</sup> photoresists,<sup>11,12</sup> lithographic printing plates,<sup>13</sup> method for ozone determination,<sup>14</sup> treatment of wastewater,<sup>15</sup> determination of silver,<sup>16</sup> nail polish,<sup>17</sup> monitoring sterilization,<sup>18</sup> determination of proteins,<sup>19</sup> induce apoptosis in cancer cells,<sup>20</sup> treatment of cancer cells,<sup>21</sup> antiHIV agent,<sup>22</sup> diagnosis and treatment of amyloidosis,<sup>23</sup> cancer chemopreventive activity,<sup>24</sup> drug design,<sup>25</sup> inhibition of influenza virus<sup>26</sup>

**Safety/Toxicity** No data available

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# Q

## QUINALDINE RED

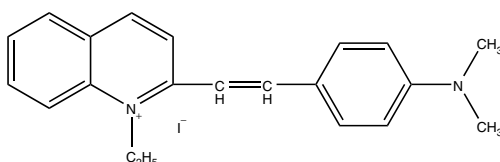
**Other Names** 2-[*p*-(Dimethylamino)styryl]-1-ethylquinolinium iodide; Quinaldine Red; Quinolinium, 2-[*p*-(dimethylamino)styryl]-1-ethyl-, iodide;  $\alpha$ -(*p*-Dimethylaminophenylethylene) quinoline ethiodide; 1-Ethyl-2-(*p*-dimethylaminostyryl)quinoline iodide; 2-(*p*-Dimethylaminostyryl) quinoline ethiodide; 2-[4-(Dimethylamino)styryl]-1-ethylquinolinium iodide; Eastman 1361

**CA Index Name** Quinolinium, 2-[2-[4-(dimethylamino)phenyl]ethenyl]-1-ethyl-, iodide

**CAS Registry Number** 117-92-0

**Merck Index Number** 8049

### Chemical Structure



**Chemical/Dye Class** Miscellaneous, Quinoline, Styryl

**Molecular Formula** C<sub>21</sub>H<sub>23</sub>N<sub>2</sub>I

**Molecular Weight** 430.33

**pH Range** 1.4–3.2

**Color Change at pH** Colorless (1.4) to red (3.2)

**pKa** 2.63

**Physical Form** Very dark red or reddish-black powder

**Solubility** Sparingly soluble in water; freely soluble in ethanol

**UV-Visible ( $\lambda_{\text{max}}$ )** 528 nm

**Melting Point** 241–243°C

**Synthesis** Synthetic methods<sup>1–4</sup>

**Major Applications** Display device,<sup>5,6</sup> photoresists,<sup>7</sup> lithographic plates,<sup>8,9</sup> toner,<sup>10</sup> paints,<sup>11</sup> coating materials,<sup>12</sup> hair dye,<sup>13</sup> treatment of mechanical allodynia,<sup>14</sup> regulation of cell proliferation,<sup>15</sup> diagnostic agents for diseases related with amyloid accumulation,<sup>16</sup> treatment of virus infectious diseases,<sup>17</sup> detecting enzyme activity,<sup>18</sup> dental bleaching materials<sup>19</sup>

**Safety/Toxicity** No data available

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19. Kutsch, V. K. Dental bleaching compositions, kits and methods. US Patent 6149895, 2000; *Chem. Abstr.* **2000**, 133, 366227.

## QUININE

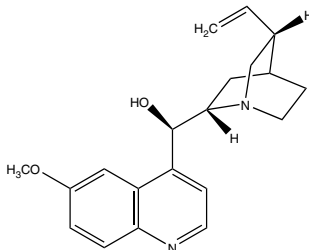
**Other Names** Quinine; (–)-Quinine; (8S,9R)-Quinine; (R)-(–)-Quinine; 6'-Methoxycinchonidine; Chinine; NSC 192949

**CA Index Name** Cinchonan-9-ol, 6'-methoxy-, (8 $\alpha$ ,9R)-

**CAS Registry Number** 130-95-0

**Merck Index Number** 8061

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Quinoline

**Molecular Formula** C<sub>20</sub>H<sub>24</sub>N<sub>2</sub>O<sub>2</sub>

**Molecular Weight** 324.42

**pH Range** 3.0–5.0;  
9.5–10.0

**Color Change at pH** Blue fluorescence (3.0) to weak violet fluorescence (5.0)

Weak violet fluorescence (9.5) to nonfluorescence (10.0)

**pKa** 5.07, 9.7

**Physical Form** White to off-white powder

**Solubility** Slightly soluble in water; soluble in ethanol, chloroform, glycerol; insoluble in petroleum ether

**Melting Point** 177°C (decompose)

**Boiling Point** 495.9 ± 40.0°C Pressure: 760 Torr


**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Bird repellents,<sup>6</sup> sunscreen,<sup>7</sup> antimalarial agent,<sup>8</sup> antiviral agent,<sup>9,10</sup> antitumor agent,<sup>11</sup> antiparasitic agent,<sup>11</sup> treatment of epilepsy,<sup>12</sup> skeletal muscle spasm,<sup>13</sup> drug-coated coronary stent system<sup>14</sup>

**Safety/Toxicity** Antimalarial drug toxicity,<sup>15</sup> cardiotoxicity,<sup>16</sup> cytotoxicity,<sup>17</sup> hepatotoxicity,<sup>17</sup> human toxicity,<sup>18</sup> ototoxicity,<sup>19</sup> phototoxicity<sup>20</sup>

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## QUININIC ACID

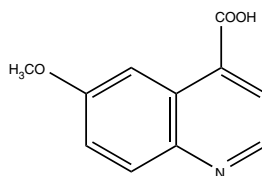
**Other Names** Cinchoninic acid, 6-methoxy-; 6-Methoxy-4-quinolinecarboxylic acid; 6-Methoxy-cinchoninic acid; NSC 403610; Quininic acid

**CA Index Name** 4-Quinolinecarboxylic acid, 6-methoxy-

**CAS Registry Number** 86-68-0

**Merck Index Number** 8062

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Quinoline

**Molecular Formula** C<sub>11</sub>H<sub>9</sub>NO<sub>3</sub>

**Molecular Weight** 203.19

**pH Range** 4.0–5.0

**Color Change at pH** Yellow fluorescent (4.0) to blue fluorescent (5.0)

**pKa** 5.53

**Physical Form** Pale yellow crystals

**Solubility** Slightly soluble in water, cold ethanol, ether

**Melting Point** 280°C (decompose)

**Boiling Point (Calcd.)** 385.4 ± 22.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–9</sup>

**Major Applications** Display device,<sup>10</sup> antihypertensive food materials,<sup>11</sup> nucleic acids,<sup>12</sup> antibacterial agent,<sup>1–7</sup> antimalarial agent<sup>9</sup>

**Safety/Toxicity** No data available

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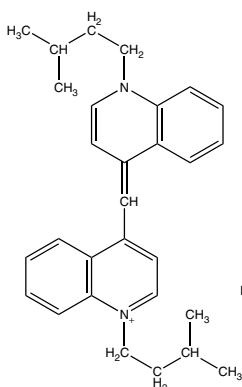
## QUINOLINE BLUE

**OtherNames** 1-Isopentyl-4-[(1-isopentyl-4(1H)-quinolylidene)methyl]-quinoliniumiodide; Cyanine blue; Quinolinium, 1-isopentyl-4-[(1-isopentyl-4(1H)-quinolylidene)methyl]-, iodide; Aquafine Blue E 1; Chinoline blue; Cyanine; Cyanine Blue 4920; Cyanine Blue GR; NK 1486; Quinoline blue  
**CA Index Name** Quinolinium, 1-(3-methylbutyl)-4-[[1-(3-methylbutyl)-4(1H)-quinolinylidene]methyl]-, iodide

**CAS Registry Number** 523-42-2

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Quinoline

**Molecular Formula** C<sub>29</sub>H<sub>35</sub>N<sub>2</sub>I

**Molecular Weight** 538.50

**pH Range** 7.0–8.0

**Color Change at pH** Colorless (7.0) to blue-violet (8.0)

**Physical Form** Green needles or crystals with dark lustre

**Solubility** Sparingly soluble in hot water; soluble in ethanol

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Display device,<sup>3</sup> semiconductors,<sup>4,5</sup> optical fibers,<sup>6</sup> antireflection films,<sup>7</sup> photoimaging process,<sup>8</sup> printed circuit board,<sup>9</sup> inks,<sup>10–12</sup> toners,<sup>13,14</sup> paints,<sup>15,16</sup> adhesives,<sup>17,18</sup> packing materials,<sup>19</sup> molding materials for fiber-reinforced plastics,<sup>20</sup> building materials,<sup>21</sup> prediction of deterioration of resins,<sup>22</sup> materials for treating animal manure<sup>23</sup>

**Safety/Toxicity** Environmental pollutants<sup>24</sup>

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# R

## RESAZURIN

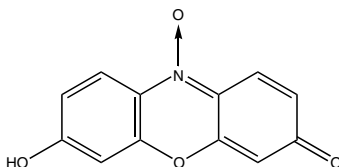
**Other Names** Resazurin; 7-Hydroxy-3H-phenoxazin-3-one 10-oxide; 7-Hydroxy-3H-phenoxazine-3-one 10-oxide; Alamar Blue; Azoresorcin; Diazaresorcinol; NSC 10438; NSC 56323; Resazoin; Resazurine; Rhodalux

**CA Index Name** 3H-Phenoxazin-3-one, 7-hydroxy-, 10-oxide

**CAS Registry Number** 550-82-3

**Merck Index Number** 8141

**Chemical Structure**



**Chemical/Dye Class** Miscellaneous, Oxazone, Heterocyclic

**Molecular Formula** C<sub>12</sub>H<sub>7</sub>NO<sub>4</sub>

**Molecular Weight** 229.19

**pH Range** 3.8–6.5

**Color Change at pH** Orange (3.8) to purple-violet (6.5)

**pKa** 6.71

**Physical Form** Dark red crystals with greenish luster

**Solubility** Insoluble in water, ether; sparingly soluble in ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 598 nm, 380 nm

**Melting Point** >250°C

**Boiling Point (Calcd.)** 477.2 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Display device,<sup>3</sup> inks,<sup>4</sup> detergents,<sup>5</sup> analysis of soil samples,<sup>6</sup> cosmetics,<sup>7</sup> measuring freshness of fruit,<sup>8</sup> sorbitol,<sup>9</sup> monitoring sugar loss,<sup>10</sup> assessment of microbials,<sup>11</sup> assays for cells,<sup>12</sup> mitochondria,<sup>13</sup> semen quality,<sup>14</sup> detecting antiviral substances,<sup>15</sup> diagnosis of bacterial and fungal infection,<sup>16</sup> treating pulmonary tuberculosis,<sup>17</sup> oral care formulation<sup>18</sup>

**Safety/Toxicity** Cytotoxicity,<sup>19</sup> chemical toxicity,<sup>20</sup> hepatotoxicity,<sup>21</sup> nephrotoxicity<sup>22</sup>

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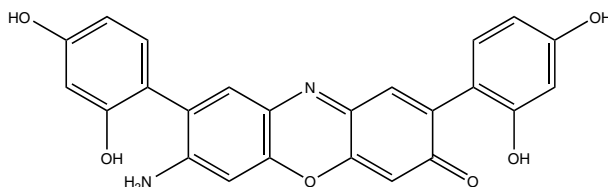
## RESORCEIN

**OtherNames** 2-Amino-3,6-bis(2,4-dihydroxyphenyl)-2-phenoxazone; Fluorescent Blue; Iris Blue B; Lacmoid; Resorcein; Resorcein Blue

**CA Index Name** 3H-Phenoxazin-3-one, 7-amino-2,8-bis(2,4-dihydroxyphenyl)-

**CAS Registry Number** 33869-21-5

**Merck Index Number** 5332

**Chemical Structure**

**Chemical/Dye Class** Miscellaneous

**Molecular Formula**  $C_{24}H_{16}N_2O_6$

**Molecular Weight** 428.39

**pH Range** 4.4–6.4

**Color Change at pH** Red (4.4) to blue (6.4)

**pKa** 5.31

**Physical Form** Black-violet powder

**Solubility** Sparingly soluble in water, ether; soluble in ethanol, methanol, amyl alcohol, acetone, acetic acid; practically insoluble in chloroform, benzene, petroleum ether

**UV-Visible** ( $\lambda_{\max}$ ) 611 nm

**Melting Point**  $>250^\circ\text{C}$

**Boiling Point (Calcd.)**  $755.3 \pm 60.0^\circ\text{C}$  Pressure: 760

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Electrochromic devices,<sup>4</sup> photosensitive materials,<sup>5</sup> parasiticides,<sup>6</sup> hair dyes,<sup>7</sup> cosmetics,<sup>8</sup> ointment for hemorrhoids<sup>9</sup>

**Safety/Toxicity** Fish toxicity<sup>10</sup>

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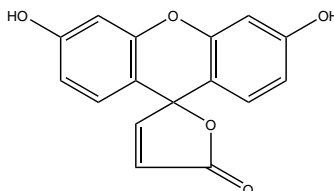
**RESORCINMALEIN**

**Other Names** Spiro[furan-2(5H),9'-xanthen]-5-one, 3',6'-dihydroxy-; Xanthene-9-acrylic acid, 3,6,9-trihydroxy-,  $\gamma$ -lactone; NSC 119894; Resorcinolmalein

**CA Index Name** Spiro[furan-2(5H),9'-[9H]xanthen]-5-one, 3',6'-dihydroxy-

**CAS Registry Number** 1227-88-9

**Merck Index Number** Not listed

**Chemical Structure****R**

**Chemical/Dye Class** Miscellaneous

**Molecular Formula** C<sub>16</sub>H<sub>10</sub>O<sub>5</sub>

**Molecular Weight** 282.25

**pH Range** 5.0–6.5

**Color Change at pH** Yellow (5.0) to orange-red (6.5)

**pKa** 5.66

**Physical Form** Yellow crystals

**Solubility** Insoluble in water, soluble in ethanol, acetone

**Melting Point** 275–276°C

**Boiling Point (Calcd.)** 610.5 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1</sup>

**Major Applications** Toner,<sup>2</sup> antiHIV agent<sup>3</sup>

**Safety/Toxicity** No data available

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## RESORUFIN

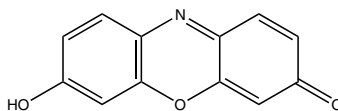
**Other Names** Resorufin; 7-Hydroxy-3H-phenoxazin-3-one; 7-Hydroxyphenoxazin-3-one; 7-Hydroxyphenoxazin-3-one; NSC 12097; Resorufine

**CA Index Name** 3H-Phenoxazin-3-one, 7-hydroxy-

**CAS Registry Number** 635-78-9

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Fluorescent, Oxazone, Heterocyclic

**Molecular Formula**  $C_{12}H_7NO_3$

**Molecular Weight** 213.19

**pH Range** 4.4–6.4

**Color Change at pH** Yellow fluorescent (4.4) to orange fluorescent (6.4)

**pKa** 6.6

**Physical Form** Purple powder

**Solubility** Sparingly soluble in water; soluble in ethanol, *N,N*-dimethylformamide

**UV-Visible ( $\lambda_{max}$ )** 573 nm, 571 nm, 585 nm, 480 nm

**Melting Point** >300°C

**Boiling Point (Calcd.)**  $413.0 \pm 45.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–4</sup>

**Major Applications** Photoelectrochemical cells,<sup>5</sup> electrochromic devices,<sup>6</sup> display device,<sup>7</sup> inks,<sup>8</sup> redox indicator,<sup>9</sup> oil product detection,<sup>10</sup> dye laser,<sup>11</sup> chemiluminescence detection,<sup>12</sup> cosmetics,<sup>13</sup> microbial fuel cells,<sup>14</sup> cytochrome P 450 assay,<sup>15</sup> multiplex assays,<sup>16</sup> analyzing cells,<sup>17</sup> semen quality,<sup>18</sup> testing prenatal abnormalities,<sup>19</sup> detecting nucleic acids,<sup>20</sup> antitumor agent<sup>21</sup>

**Safety/Toxicity** Toxicity,<sup>22</sup> mutagenicity<sup>23</sup>

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## RHODOL GREEN

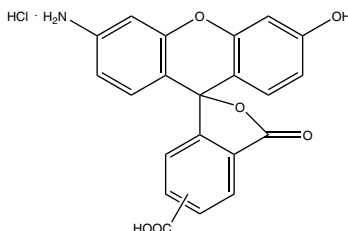
**Other Names** Rhodol Green carboxylic acid, hydrochloride 5(6)-CRF 492

**CA Index Name** Rhodol Green

**CAS Registry Number** 183185-51-5

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent

**Molecular Formula**  $C_{21}H_{14}ClNO_6$

**Molecular Weight** 411.80

**pH Range** 5.0–7.8

**Color Change at pH** Weak green fluorescence (5.0) to strong green fluorescence (7.8)

**pKa** 5.6

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in *N,N*-dimethylformamide

**UV-Visible** ( $\lambda_{max}$ ) 480 nm

**Melting Point** >250°C

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Optical sensors,<sup>2</sup> determining the size of polynucleotides,<sup>3</sup> diagnosis of parathyroid carcinoma,<sup>4</sup> genetic diseases,<sup>5</sup> detecting multiple nucleic acid targets,<sup>6</sup> antitumor agent<sup>7</sup>

**Safety/Toxicity** No data available

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**p-ROSOLIC ACID**

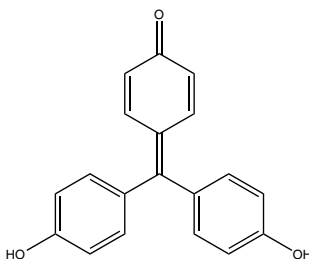
**Other Names** 2,5-Cyclohexadien-1-one, 4-[bis(p-hydroxyphenyl)methylene]-; Aurin; 4,4'-Dihydroxyfuchson; 4-(p,p'-Dihydroxybenzhydrylidene)-2,5-cyclohexadien-1-one; 4-[Bis(p-hydroxyphenyl)methylene]-2,5-cyclohexadien-1-one; Aurin 555; Aurine; C.I. 43800; Corallin; Corallin Spirit Soluble; NSC 7805; Pararosolic acid; Rosalic acid; Spirit Aurine; p-Rosolic acid

**CA Index Name** 2,5-Cyclohexadien-1-one, 4-[bis(4-hydroxyphenyl)methylene]-

**CAS Registry Number** 603-45-2

**Merck Index Number** 881

**Chemical Structure**



**Chemical/Dye Class** Triphenylmethane

**Molecular Formula** C<sub>19</sub>H<sub>14</sub>O<sub>3</sub>

**Molecular Weight** 290.31

**pH Range** 6.6–8.0

**Color Change at pH** Yellow (6.6) to red (8.0)

**pKa** 6.98

**Physical Form** Red crystals

**Solubility** Practically insoluble in water, benzene; freely soluble in ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 534.6 nm, 479.5 nm, 482 nm

**Melting Point** 309°C (decompose)

**Boiling Point (Calcd.)** 543.0 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–9</sup>

**Major Applications** Antireflective coatings,<sup>10</sup> thermochromic materials,<sup>11</sup> photoresists,<sup>2</sup> electrorheological materials,<sup>12</sup> film patterning,<sup>13</sup> recording materials,<sup>14</sup> lithium battery,<sup>15</sup> semiconductors,<sup>16</sup> printing materials,<sup>17</sup> inks,<sup>18</sup> corrosion inhibitors,<sup>19</sup> adhesives,<sup>20</sup> drugs,<sup>21</sup> detecting viable cells,<sup>22</sup> treatment of Alzheimer's disease<sup>1</sup>

**Safety/Toxicity** Toxic activity,<sup>23</sup> environmental toxicity,<sup>24</sup> cytopathogenicity<sup>25</sup>

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## RUBROPHEN

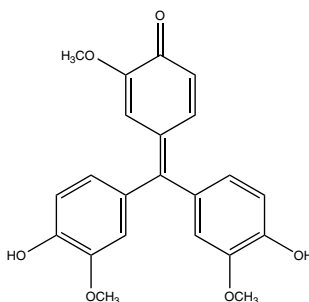
**Other Names** Rubrophen; NSC 71806; Rubrocol

**CA Index Name** 2,5-Cyclohexadien-1-one, 4-[bis(4-hydroxy-3-methoxyphenyl)-methylene]-2-methoxy-

**CAS Registry Number** 5664-34-6

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Triphenylmethane

**Molecular Formula** C<sub>22</sub>H<sub>20</sub>O<sub>6</sub>

**Molecular Weight** 380.39

**pH Range** 1.0–3.0;

6.5–7.2

**Color Change at pH** Cherry-red (1.0) to yellow (3.0)

Yellow (6.5) to violet (7.2)

**pKa** 3.0, 4.4, 10.0

**Physical Form** Solid

**Solubility** Slightly soluble in water; soluble in ethanol

**Melting Point** 251°C

**Boiling Point (Calcd.)** 646.1 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–7</sup>

**Major Applications** Pharmaceutical,<sup>8</sup> fungicides,<sup>9</sup> treatment of tuberculosis<sup>10</sup>

**Safety/Toxicity** No data available

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# S

## SALICYLALDEHYDE SEMICARBAZONE

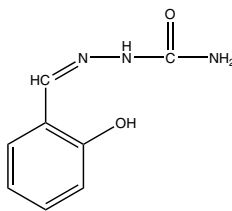
**Other Names** Salicylaldehyde, semicarbazone; 2-Hydroxybenzaldehyde semicarbazone; NSC 1604

**CA Index Name** Hydrazinecarboxamide, 2-[(2-hydroxyphenyl)methylene]-

**CAS Registry Number** 3030-97-5

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>8</sub>H<sub>9</sub>N<sub>3</sub>O<sub>2</sub>

**Molecular Weight** 179.18

**pH Range** 7.6–8.0

**Color Change at pH** Yellow fluorescence (7.6) to blue fluorescence (8.0)

**pKa** 7.75

**Physical Form** Solid

**Solubility** Insoluble in water; soluble in ethanol

**Melting Point** 227–228°C

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Electroluminescent devices,<sup>6</sup> semiconductor wafer,<sup>7</sup> corrosion inhibitors,<sup>8</sup> antibacterial agent,<sup>1</sup> anticonvulsant agent,<sup>9</sup> anticancer agent<sup>10</sup>

**Safety/Toxicity** No data available

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## SALICYLIC ACID

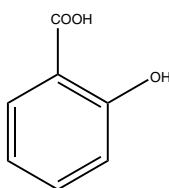
**Other Names** 171; 2-Carboxyphenol; 2-Hydroxybenzenecarboxylic acid; 2-Hydroxybenzoic acid; 311; 334; 337; 380; 51; Advanced Pain Relief Callus Removers; Advanced Pain Relief Corn Removers; Clear away Wart Remover; Compound W; Dr. Scholl's Callus Removers; Dr. Scholl's Corn Removers; Dr. Scholl's Wart Remover Kit; Duofil Wart Remover; Duoplant; Freezone; Ionil; Ionil Plus; K 537; K 557; NSC 180; Phenol-2-carboxylic acid; Psoriacid-S-Stift; Retarder W; Rutranex; Salicylic Acid Soap; Salicylic acid collodion; Saligel; Salonil; Stri-Dex; Trans-Ver-Sal; *o*-Carboxyphenol; *o*-Hydroxybenzoic acid

**CA Index Name** Benzoic acid, 2-hydroxy-

**CAS Registry Number** 69-72-7

**Merck Index Number** 8332

### Chemical Structure



**Chemical/Dye Class** Fluorescent

**Molecular Formula** C<sub>7</sub>H<sub>6</sub>O<sub>3</sub>

**Molecular Weight** 138.12

**pH Range** 2.5–4.0

**Color Change at pH** Nonfluorescence (2.5) to dark blue fluorescence (4.0)

**pKa** 2.98

**Physical Form** White crystals

**Solubility** Slightly soluble in water; soluble in ethanol, acetone

**UV-Visible** ( $\lambda_{\text{max}}$ ) 210 nm, 234 nm, 303 nm

**Melting Point** 159°C

**Boiling Point** 211°C

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Semiconductors,<sup>6,7</sup> nanoparticles,<sup>8</sup> photoresists,<sup>9</sup> lubricating oils,<sup>10</sup> UV absorbers,<sup>11</sup> adhesive,<sup>12</sup> leather,<sup>13</sup> cleaner,<sup>14</sup> hair dye,<sup>15</sup> soaps,<sup>16</sup> cosmetics,<sup>17</sup> pain medication,<sup>18</sup> analgesics,<sup>19</sup> antibacterial agent,<sup>20</sup> treatment of dandruff,<sup>21</sup> hyperpigmented skin,<sup>22</sup> tinea pedis,<sup>23</sup> onychomycosis,<sup>24</sup> osteoporosis,<sup>25</sup> beriberi,<sup>26</sup> fungicidal skin disease,<sup>27</sup> autoimmune disease<sup>28</sup>

**Safety/Toxicity** Acute toxicity,<sup>29</sup> aquatic toxicity,<sup>30</sup> carcinogenicity,<sup>31</sup> cytotoxicity,<sup>32</sup> ecotoxicity,<sup>33</sup> environmental toxicity,<sup>34</sup> hemotoxicology,<sup>35</sup> mutagenicity,<sup>36</sup> safety assessment<sup>37</sup>

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## SALICYL YELLOW

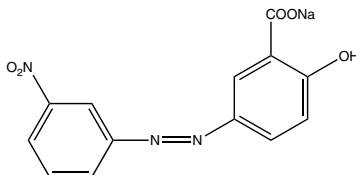
**Other Names** C.I. Mordant Yellow 1; C.I. Mordant Yellow 1, monosodium salt; Salicylic acid, 5-(*m*-nitrophenylazo)-, sodium salt; Acid Chrome Yellow 2GW; Acid Chrome Yellow GG; Alizarin Yellow; Alizarin Yellow G; Alizarin Yellow G sodium salt; Alizarin Yellow GG; Alizarine Yellow 2G; Alizarine Yellow AGP; Alizarine Yellow G; Alizarine Yellow GG; Alizarine Yellow GGW; Alizarine Yellow GM; Alizarine Yellow GR; Alizarol Yellow GW; Anthranol Chrome Yellow 2G; Anthranol Chrome Yellow 5GS; Atlantichrome Yellow 2G; Azochromol Yellow 5G; C.I. 14025; Calcochrome Yellow 2G; Chrome Fast Yellow RW; Chrome Yellow 2G; Chrome Yellow 2GR; Chromol Yellow G; Chromol Yellow N; Cromal Yellow M; Eniacromo Yellow G; Eriochromal Yellow 2G; Eriochrome Yellow 2G; Eriochrome Yellow GS; Fenakrom Yellow R; Hidachrome Yellow 2G; Hispacrom Yellow 2G; Hispacrom Yellow 2GR; Java Chrome Yellow GT; Java Unichrome Yellow GT; Kayaku Mordant Yellow GG; Magracrom Yellow GG; Metachrome Yellow; Metachrome Yellow RA; Metomega Chrome Yellow GM; Mitsui Chrome Yellow GG; Monochrome Yellow MG; Orthochrome Yellow GGW; Pontachrome Yellow GS; RV 1; Salicyl yellow; Salicylic acid, (*m*-nitrophenylazo)-, sodium salt; Showa Chrome Yellow GG; Sodium 5-(*m*-nitrophenylazo) salicylate; Sodium 5-[(3-nitrophenyl)-azo]-salicylate; Sodium *m*-nitrobenzeneazosalicylate; Solochrome Yellow WN; Sunchromine Yellow GG; Yodochrome Yellow GGN

**CA Index Name** Benzoic acid, 2-hydroxy-5-[(3-nitrophenyl)azo]-, monosodium salt

**CAS Registry Number** 584-42-9

**Merck Index Number** 5919

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{13}H_8N_3O_5Na$

**Molecular Weight** 309.22

**pH Range** 10.0–12.0

**Color Change at pH** Yellow (10.0) to orange (12.0)

**Physical Form** Yellow-orange powder

**Solubility** Soluble in water, methyl cellosolve; slightly soluble in ethanol, acetone

**UV-Visible** ( $\lambda_{max}$ ) 362 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Optical engineering applications,<sup>4</sup> sensors,<sup>5</sup> making masks,<sup>6</sup> electrorheological materials,<sup>7</sup> surface treatment of copper,<sup>8</sup> coloring zinc,<sup>9</sup> aluminum,<sup>10</sup> corrosion testing,<sup>11</sup> adhesive,<sup>12</sup> lubricants,<sup>13</sup> textiles,<sup>14</sup> food storage,<sup>15</sup> determine bacterial growth,<sup>16</sup> pharmaceutical preparations<sup>17</sup>

**Safety/Toxicity** Mutagenicity<sup>18</sup>

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## SOLOCHROME VIOLET RS

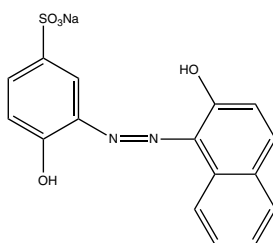
**Other Names** C.I. Mordant Violet 5; C.I. Mordant Violet 5, monosodium salt; Eriochrome Violet B; Acid Alizarin Violet N; Acid Alizarine Violet; Acid Alizarine Violet B; Acid Chrome Violet K; Acid Chrome Violet N; Aizen Chrome Violet BH; Alizarine Violet N; Alphacroic Violet B; Atlantichrome Violet B; Brasilan Chrome Violet B; C.I. 15670; Chromacid Violet R; Chromaven Violet B; Chrome Fast Violet B; Chrome Violet B; Chrome Violet K; Chrome Violet R; Cromal Violet B; Diacromo Violet N; Diamond Corinth N; Durochrome Violet B; Erio Chrome Violet BA; Erio Chrome Violet BR; Hispacrom Violet B; Java Chrome Violet B; Magracrom Violet N; Mitsui Chrome Violet BC; Monochrome Violet B; Mordant Violet 5; Omega Chrome Dark Violet D; Pontachrome Violet SW; Solochrome Violet; Solochrome Violet R; Solochrome Violet RS; Solocrom Violet RS; Sunchromine Violet B; Superchrome Violet B; Symulon Chrome Violet B; Tertrochrome Violet N; Yodochrome Violet B

**CA Index Name** Benzenesulfonic acid, 4-hydroxy-3-[(2-hydroxy-1-naphthalenyl)azo]-, monosodium salt

**CAS Registry Number** 2092-55-9

**Merck Index Number** Not listed

**Chemical Structure**



**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{16}H_{11}N_2O_5SNa$

**Molecular Weight** 366.33

**pH Range** 6.5–9.0

**Color Change at pH** Orange-red (6.5) to violet (9.0)

**pKa** 4.35, 7.4, 9.35

**Physical Form** Reddish-violet crystals

**Solubility** Soluble in water, ethanol

**UV-Visible** ( $\lambda_{max}$ ) 501 nm

**Melting Point** >300°C

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** inks,<sup>4</sup> dye lasers,<sup>5</sup> in manufacture of vinyl polymers,<sup>6</sup> textiles<sup>1</sup> determination of iron,<sup>7</sup> calcium,<sup>8</sup> aluminum,<sup>9–11</sup> tantalum,<sup>12</sup> monitoring hardness in industrial water,<sup>13</sup> measuring chlorine dioxide in drinking water,<sup>14</sup> hypoglycemic agents,<sup>15</sup> nuclear fluorochrome<sup>16</sup>

**Safety/Toxicity** Mutagenicity<sup>17</sup>

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## SULPHAN BLUE

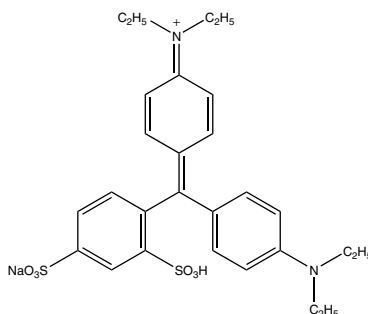
**Other Names** C.I. Acid Blue 1, sodium salt; Ethanaminium, *N*-[4-[[4-(diethylamino)phenyl](2,4-disulfophenyl)methylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-, hydroxide, inner salt, sodium salt; Xylene Blue VS; [4-[ $\alpha$ -[*p*-(Diethylamino)phenyl]-2,4-isulfobenzylidene]-2,5-cyclohexadien-1-ylidene]-diethylammonium hydroxide, inner salt, sodium salt; 1085 Blue; Acid Blue 1; Acid Blue V; Acid Bright Azure Z; Acid Brilliant Blue Z; Acid Brilliant Sky Blue Z; Acid Leather Blue V; Acid Turquoise Blue V; Aizen Brilliant Acid Pure Blue VH; Alphazurine 2G; Amacid Blue V; Bleu Patente V; Blue URS; Blue VRS; Brilliant Acid Blue A Export; Brilliant Acid Blue V Extra; Brilliant Acid Blue VS; Brilliant Blue GS; Bucacid Patent Blue VF; C.I. 42045; C.I. Acid Blue 1; C.I. Food Blue 3; Carmine Blue VF; Disulfine blue VN; Disulphine Blue VN; Disulphine Blue VN 150; Disulphine VN; Duasyn Acid Blue V 02; Edicol Supra Blue VR; Erioglaurine supra; Fenazo Blue XF; Hexacol Blue VRS; Hidacid Blue V; Kiton Pure Blue V; Kiton Pure Blue V.FQ; Leather Blue G; Merantine Blue VF; Orient Water Blue 106; Patent Blue; Patent Blue V; Patent Blue VF; Patent Blue VF Special; Patent Blue VF-CF; Patent Pure Blue VX; Patent blue VS; Patent blue violet; Pontacyl Brilliant Blue V; Sodium Blue VRS; Sodium Patent Blue V; Sulfan blue; Sulphan Blue; Sumitomo Patent Pure Blue VX; Tertracid Carmine Blue V

**CA Index Name** Ethanaminium, *N*-[4-[[4-(diethylamino)phenyl](2,4-disulfophenyl)methylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-, inner salt, sodium salt

**CAS Registry Number** 129-17-9

**Merck Index Number** 8987

**Chemical Structure**



**Chemical/Dye Class** Triphenylmethane

**Molecular Formula**  $C_{27}H_{31}N_2O_6S_2Na$

**Molecular Weight** 566.68

**pH Range** 0.8–3.0

**Color Change at pH** Yellow-orange (0.8) to deep blue (3.0)

**Physical Form** Dark blue powder

**Solubility** Soluble in water; partly soluble in ethanol; insoluble in xylene

**UV-Visible** ( $\lambda_{max}$ ) 635 nm, 410 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1-3</sup>

**Major Applications** Liquid crystal displays,<sup>4</sup> color filters,<sup>5,6</sup> electrorheological materials,<sup>7</sup> photographic materials,<sup>8</sup> optical filters,<sup>9</sup> inks,<sup>10</sup> highlighters,<sup>11</sup> dyeing paper,<sup>12</sup> wood dyeing,<sup>13</sup> textiles,<sup>14</sup> detergents,<sup>15</sup> hair dyes,<sup>16</sup> cosmetics,<sup>17</sup> lymph node identification,<sup>18</sup> antiparasitic agent,<sup>19</sup> nanocomposite particles for biomedical applications<sup>20</sup>

**Safety/Toxicity** Acute toxicity,<sup>21</sup> genotoxicity,<sup>22</sup> mutagenicity,<sup>23,24</sup> allergic reaction,<sup>25</sup> adverse reaction<sup>26</sup>

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# T

## TETRABROMOPHENOL BLUE

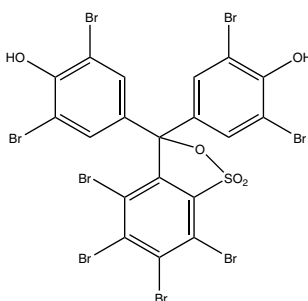
**Other Names** Phenol, 4,4'-(4,5,6,7-tetrabromo-3H-2,1-benzoxathiol-3-ylidene)-bis[2,6-dibromo-, S,S-dioxide; 3H-2,1-Benzoxathiole, phenol derivative; NSC 11236; Tetrabromphenol blue

**CA Index Name** Phenol, 4,4'-(4,5,6,7-tetrabromo-1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-

**CAS Registry Number** 4430-25-5

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>19</sub>H<sub>6</sub>Br<sub>8</sub>O<sub>5</sub>S

**Molecular Weight** 985.54

**pH Range** 3.0–4.6

**Color Change at pH** Yellow (3.0) to blue (4.6)

**pKa** 3.69

**Physical Form** Off-white to pale lavender powder

**Solubility** Soluble in water, ethanol, methanol, acetone, acetic acid

**UV-Visible** ( $\lambda_{\text{max}}$ ) 610 nm, 388 nm

**Melting Point** 204°C (decompose)

**Boiling Point (Calcd.)** 728.8 ± 60.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Semiconductors,<sup>3</sup> thin films,<sup>4</sup> recording materials,<sup>5</sup> chemically amplified resists,<sup>6</sup> photography,<sup>7</sup> lithographic plates,<sup>8</sup> inks,<sup>9</sup> toners,<sup>10</sup> detergents,<sup>11</sup> hair dyes,<sup>12</sup> diapers,<sup>13</sup> detecting proteins,<sup>14,15</sup> contact lens,<sup>16</sup> urine analysis test strips,<sup>17</sup> distinguishing between allergies and infections<sup>18</sup>

**Safety/Toxicity** Mutagenicity<sup>19</sup>

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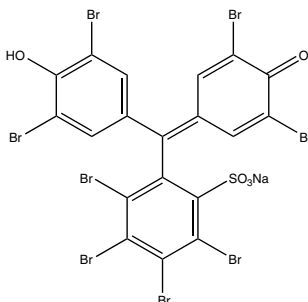
**TETRABROMOPHENOL BLUE, SODIUM SALT**

**Other Names** Phenol, 4,4'-(4,5,6,7-tetrabromo-3H-2,1-benzoxathiol-3-ylidene)-bis[2,6-dibromo-, S,S-dioxide, monosodium salt; 3H-2,1-Benzoxathiole, phenol derivative; Tetrabromophenol Blue monosodium salt

**CA Index Name** Phenol, 4,4'-(4,5,6,7-tetrabromo-1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-, monosodium salt

**CAS Registry Number** 108321-10-4

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>19</sub>H<sub>5</sub>Br<sub>8</sub>O<sub>5</sub>SNa

**Molecular Weight** 1007.58

**pH Range** 3.0–4.6

**Color Change at pH** Yellow (3.0) to blue (4.6)

**pKa** 5.69

**Physical Form** Dark brown crystals

**Solubility** Soluble in water, ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 610 nm

**Melting Point** >250°C

**Synthesis** Synthetic method<sup>1,2</sup>

**Major Applications** Chemically amplified resists<sup>3,4</sup>

**Safety/Toxicity** No data available

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2. Orndorff, W. R.; Sherwood, F. W. Phenolsulfonephthalein and some of its derivatives. *J. Am. Chem. Soc.* **1923**, *45*, 486–500.
3. Kim, J.; Kwon, Y.; Yun, H.; Jung, M. Post-exposure delay effect in chemically amplified resists. *J. Photopolym. Sci. Technol.* **2001**, *14*, 401–406.
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## TETRABROMOPHENOLPHTHALEIN

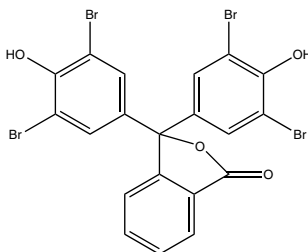
**Other Names** Phenolphthalein, 3',3'',5',5''-tetrabromo-; 3',3'',5',5''-Tetrabromophenolphthalein;  
A 84568; NSC 21261; Tetrabromophenolphthalein

**CA Index Name** 1(3H)-Isobenzofuranone, 3,3-bis(3,5-dibromo-4-hydroxyphenyl)-

**CAS Registry Number** 76-62-0

**Merck Index Number** 9186

### Chemical Structure



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**Chemical/Dye Class** Phthalein

**Molecular Formula**  $C_{20}H_{10}Br_4O_4$

**Molecular Weight** 633.91

**pH Range** 7.6–9.4

**Color Change at pH** Colorless (7.6) to violet (9.4)

**pKa** 6.20

**Physical Form** White powder

**Solubility** Practically insoluble in water; soluble in ethanol, ether

**UV-Visible ( $\lambda_{max}$ )** 310 nm, 218 nm

**Melting Point** 296°C

**Boiling Point (Calcd.)** 598.6  $\pm$  50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Optical materials,<sup>4</sup> photoresists,<sup>5,6</sup> photoreceptor materials,<sup>7</sup> photoconductive materials,<sup>8</sup> inks,<sup>9,10</sup> genomics,<sup>11</sup> diagnosis of kidney diseases<sup>12</sup>

**Safety/Toxicity** No data available

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## TETRAIODOPHENOLSULFONEPHTHALEIN

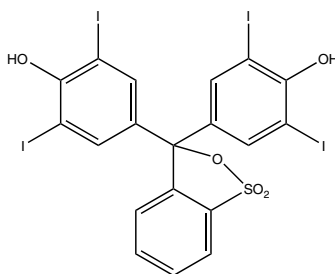
**Other Names** Iodophenol blue; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2,6-diiodo-, *S*, *S*-dioxide; 3H-2,1-Benzoxathiole, phenol derivative; NSC 36792

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2,6-diiodo-

**CAS Registry Number** 4430-24-4

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>19</sub>H<sub>10</sub>I<sub>4</sub>O<sub>5</sub>S

**Molecular Weight** 857.96

**pH Range** 3.0–4.8

**Color Change at pH** yellow (3.0) to blue (4.8)

**pKa** 4.16

**Physical Form** Brown powder

**Solubility** Slightly soluble in water; soluble in ethanol, methanol, acetone, ether, acetic acid

**UV-Visible** ( $\lambda_{\text{max}}$ ) 433 nm

**Melting Point** 229°C (decompose)

**Boiling Point (Calcd.)** 615.3 ± 55.0°C Pressure: 760 Torr

**Synthesis** Synthetic method<sup>1</sup>

**Major Applications** Shelf life indicator,<sup>2</sup> determining proteins,<sup>3</sup> human serum albumins,<sup>4</sup> polymeric biguanides,<sup>5</sup> examining renal and hepatic functions,<sup>6</sup> apoptosis assay<sup>7</sup>

**Safety/Toxicity** No data available

### References

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## TETRYL

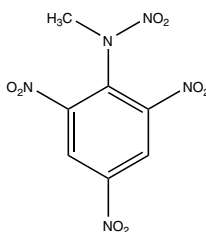
**Other Names** Aniline, *N*-methyl-*N*,2,4,6-tetranitro-; 2,4,6-*N*-Tetranitro-*N*-methylaniline; 2,4,6-Tetryl; 2,4,6-Trinitro-*N*-methyl-*N*-nitroaniline; 2,4,6-Trinitrophenyl-*N*-methylnitramine; 2,4,6-Trinitrophenylmethylnitroamine; CE; *N*-Methyl-*N*,2,4,6-tetranitroaniline; *N*-Methyl-*N*-picrylnitramine; *N*-Picryl-*N*-methylnitramine; NSC 2166; Nitramine; Nitramine (indicator); Picrylmethylnitramine; Picrylnitromethylamine; Tetralit; Tetralite; Tetril; Tetryl

**CA Index Name** Benzenamine, *N*-methyl-*N*,2,4,6-tetranitro-

**CAS Registry Number** 479-45-8

**Merck Index Number** 6573

### Chemical Structure



**Chemical/Dye Class** Nitro

**Molecular Formula** C<sub>7</sub>H<sub>5</sub>N<sub>5</sub>O<sub>8</sub>

**Molecular Weight** 287.14

**pH Range** 10.8–13.0

**Color Change at pH** Colorless (10.8) to red-brown (13.0)

**pKa** 12.66

**Physical Form** Yellow crystals

**Solubility** Insoluble in water; soluble in ethanol, ether, benzene, acetic acid

**Melting Point** 130–132°C

**Boiling Point (Calcd.)** 503.7 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–11</sup>

**Major Applications** Explosives,<sup>2,3,9–17</sup> paints,<sup>18</sup> food storage<sup>19</sup>

**Safety/Toxicity** Cytotoxicity,<sup>20</sup> marine toxicity,<sup>21</sup> mutagenicity,<sup>22,23</sup> genotoxicity<sup>24</sup>

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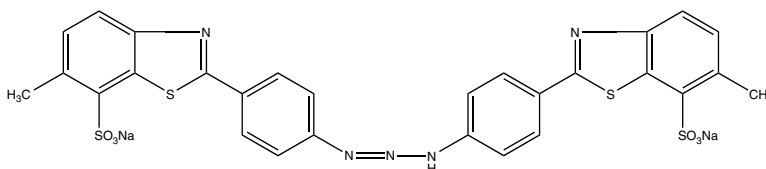
## THIAZOL YELLOW G

**Other Names** C.I. Direct Yellow 9; C.I. Direct Yellow 9, disodium salt; Clayton Yellow; Atlantic Brilliant Yellow MN; Benzo Yellow TZ; C.I. 19540; Chlorazol Yellow 2G; Chlorazol Yellow DP; Diaphtamine Brilliant Yellow 6GS; Diazamine Golden Yellow T; Diazol Yellow J; Direct Yellow MTZ; Direct Yellow TZ; Ferro 42-145A; Hispamin Pure Yellow T2G; Mimosa Z; Peeramine Bright Yellow MN; Pontamine Pure Yellow; Pontamine Pure Yellow MN; Thiazol Yellow; Thiazol Yellow G; Thiazol Yellow GGM; Thiazol Yellow R; Thiazol Yellow Z; Thiazole Y; Thiazole Yellow G; Thiazole Yellow GGM; Thiazole yellow; Titan Yellow; Titan Yellow Dye; Titan Yellow G

**CA Index Name** 7-Benzothiazolesulfonic acid, 2,2'-(1-triazene-1,3-diyl-di-4,1-phenylene)bis [6-methyl-, disodium salt

**CAS Registry Number** 1829-00-1

**Merck Index Number** 9310

**Chemical Structure**

**Chemical/Dye Class** Azo, thiazole

**Molecular Formula** C<sub>28</sub>H<sub>19</sub>N<sub>5</sub>O<sub>6</sub>S<sub>4</sub>Na<sub>2</sub>

**Molecular Weight** 695.73

**pH Range** 11.0–13.0

**Color Change at pH** Yellow (11.0) to red (13.0)

**Physical Form** Yellowish-brown powder

**Solubility** Soluble in water, ethanol

**UV-Visible (λ<sub>max</sub>)** 402 nm

**Melting Point** >250°C

**Synthesis** Synthetic methods<sup>1–4</sup>

**Major Applications** Display device,<sup>5</sup> optical sensors,<sup>6,7</sup> thin-film device,<sup>8</sup> incandescent electric lamps,<sup>9</sup> photoreceptors,<sup>10</sup> lithographic process,<sup>11</sup> inks,<sup>12</sup> pencil leads,<sup>13</sup> paints,<sup>14</sup> adhesives,<sup>15</sup> plastic materials,<sup>16</sup> molding materials,<sup>17</sup> steel plates,<sup>18</sup> detection of albumin,<sup>19</sup> treatment of amyloidosis disorders,<sup>20</sup> treatment of apolipoprotein E-related diseases<sup>21</sup>

**Safety/Toxicity** Eye irritation test<sup>22</sup>

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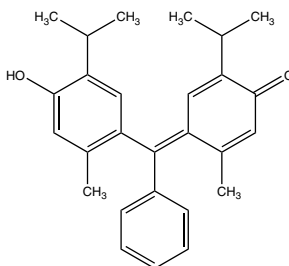
**THYMOLBENZEIN**

**Other Names** *p*-Mentha-1,4-dien-3-one, 6-[ $\alpha$ -(5-hydroxycarvacryl)benzylidene]; Thymolbenzein

**CA Index Name** 2,5-Cyclohexadien-1-one, 4-[[4-hydroxy-2-methyl-5-(1-methylethyl)phenyl]phenylmethylene]-5-methyl-2-(1-methylethyl)-

**CAS Registry Number** 5811-49-4

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Benzein

**Molecular Formula** C<sub>27</sub>H<sub>30</sub>O<sub>2</sub>

**Molecular Weight** 386.53

**pH Range** 1.5–2.5

7.6–9.0

**Color Change at pH** Red (1.5) to yellow (2.5)

Yellow (7.6) to blue (9.0)

**pKa** 3.3, 3.5, 13.15, 13.9

**Physical Form** Bright red powder

**Solubility** Insoluble in water; soluble in ethanol, methanol, acetone, acetic acid

**Melting Point** 184°C

**Boiling Point (Calcd.)** 548.0 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Applications** Indicator<sup>3</sup>

**Safety/Toxicity** No data available

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## THYMOL BLUE

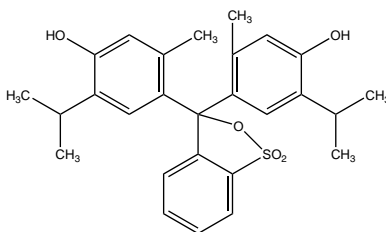
**Other Names** Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[5-methyl-2-(1-methylethyl)-, *S,S*-dioxide; Thymol, 6,6'-(3H-2,1-benzoxathiol-3-ylidene)di-, *S,S*-dioxide; Thymolsulfonephthalein; 3H-2,1-Benzoxathiole, phenol derivative; NSC 11238; Thymol blue; Thymolsulfophthalein

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[5-methyl-2-(1-methylethyl)-

**CAS Registry Number** 76-61-9

**Merck Index Number** 9400

**Chemical Structure**



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>27</sub>H<sub>30</sub>O<sub>5</sub>S

**Molecular Weight** 466.59

**pH Range** 1.2–2.8;

8.0–9.6

**Color Change at pH** Red (1.2) to yellow (2.8)

Yellow (8.0) to blue (9.6)

**pKa** 1.65, 8.90

**Physical Form** Dark bluish-green to brownish powder

**Solubility** Insoluble in water; soluble in ethanol, methanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 594 nm, 376 nm, 544 nm, 430 nm

**Melting Point** 223°C (decompose)

**Boiling Point (Calcd.)** 580.5 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–8</sup>

**Major Applications** Display device,<sup>9</sup> semiconductors,<sup>10</sup> sensors,<sup>11</sup> fuel cells,<sup>12</sup> antimisting coating for glass,<sup>13</sup> toys,<sup>14</sup> corrosion inhibitor,<sup>15</sup> multi-level alert system,<sup>16</sup> correction fluid,<sup>17</sup> textiles,<sup>18</sup> falsification-proof security paper,<sup>19</sup> packaging system,<sup>20</sup> measurement of hydrogen ion concentration in swimming pool water,<sup>21</sup> humidity-indicating agent,<sup>22</sup> diapers,<sup>23</sup> cosmetics,<sup>24</sup> biostatic materials,<sup>25</sup> determine bacteria growth,<sup>26</sup> psychoactive drugs,<sup>27</sup> antidepressant drugs,<sup>28</sup> dental impression material<sup>29</sup>

**Safety/Toxicity** Mutagenicity<sup>30</sup>

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## THYMOLPHTHALEIN

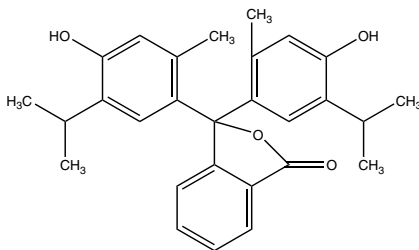
**Other Names** Phenolphthalein, 5',5''-diisopropyl-2',2''-dimethyl-; Thymolphthalein; 2',2''-Diisopropyl-5',5''-dimethylphenolphthalein; 3,3-Bis(4-hydroxy-3-isopropyl-6-methyl)phthalide; NSC 2186

**CA Index Name** 1(3H)-Isobenzofuranone, 3,3-bis[4-hydroxy-2-methyl-5-(1-methylethyl)phenyl]-

**CAS Registry Number** 125-20-2

**Merck Index Number** 9401

### Chemical Structure



**Chemical/Dye Class** Phthalein

**Molecular Formula** C<sub>28</sub>H<sub>30</sub>O<sub>4</sub>

**Molecular Weight** 430.54

**pH Range** 9.3–10.5

**Color Change at pH** Colorless (9.3) to blue (10.5)

**pKa** 9.70, 10.0

**Physical Form** White powder

**Solubility** Insoluble in water; soluble in ethanol, acetone

**UV-Visible** ( $\lambda_{\text{max}}$ ) 592 nm, 396 nm, 598 nm

**Melting Point** 253°C

**Boiling Point (Calcd.)** 571.6 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–7</sup>

**Major Applications** Display device,<sup>8,9</sup> semiconductors,<sup>10</sup> recording materials,<sup>11</sup> photoconductors,<sup>12</sup> sol-gel matrix,<sup>13</sup> tin electroplating process,<sup>14</sup> counterfeit-proof paper,<sup>15</sup> authentication system for secure documents,<sup>16</sup> inks,<sup>17,18</sup> pencil leads,<sup>19</sup> correction fluid,<sup>20</sup> paints,<sup>21</sup> petroleum marker,<sup>1,22</sup> tennis ball,<sup>23</sup> adhesives,<sup>24</sup> floor coatings,<sup>25</sup> textiles,<sup>26</sup> detergents,<sup>27</sup> insecticide,<sup>28</sup> lotion,<sup>29</sup> cleaning pads,<sup>30</sup> food storage,<sup>31</sup> determine bacterial growth,<sup>32</sup> Streptococci in saliva,<sup>33</sup> dental impression materials<sup>34</sup>

**Safety/Toxicity** Toxicity<sup>35</sup>

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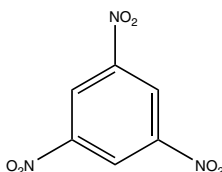
## TRINITROBENZENE

**Other Names** 1,3,5-Trinitrobenzene; 2,4,6-Trinitrobenzene; NSC 36931; TNB; TNB (nitro compound); Trinitrobenzene; *s*-Trinitrobenzene; sym-Trinitrobenzene

**CA Index Name** Benzene, 1,3,5-trinitro-

**CAS Registry Number** 99-35-4

**Merck Index Number** 9726

**Chemical Structure**

**Chemical/Dye Class** Nitro

**Molecular Formula** C<sub>6</sub>H<sub>3</sub>N<sub>3</sub>O<sub>6</sub>

**Molecular Weight** 213.10

**pH Range** 11.5–14.0

**Color Change at pH** Colorless (11.5) to orange (14.0)

**Physical Form** Light yellow crystals

**Solubility** Slightly soluble in water; soluble in ethanol

**Melting Point** 122.5°C

**Boiling Point** 315°C

**Synthesis** Synthetic methods<sup>1–8</sup>

**Applications** Explosive,<sup>9–13</sup> high-energy propellants,<sup>14</sup> energetic materials,<sup>15</sup> display device,<sup>16</sup> electroluminescent materials,<sup>17</sup> lithium batteries,<sup>18</sup> paints,<sup>19</sup> adhesives<sup>20</sup>

**Safety/Toxicity** Cytotoxicity,<sup>21</sup> carcinogenicity,<sup>22</sup> chronic toxicity,<sup>23</sup> environmental toxicity,<sup>24</sup> genotoxicity,<sup>25</sup> hazardous substance,<sup>26</sup> hematological effects,<sup>27</sup> immunotoxicity,<sup>28</sup> marine toxicity,<sup>29</sup> mutagenicity,<sup>30</sup> neurotoxicity,<sup>31</sup> phytotoxicity,<sup>32</sup> soil toxicity,<sup>33</sup> testicular effects<sup>34</sup>

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## TRINITROBENZOIC ACID

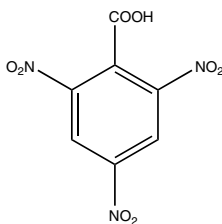
**Other Names** 1-Carboxy-2,4,6-trinitrobenzene; 2,4,6-Trinitrobenzoic acid; NSC 133453; TNBA; Trinitrobenzoic acid; sym-Trinitrobenzoic acid

**CA Index Name** Benzoic acid, 2,4,6-trinitro-

**CAS Registry Number** 129-66-8

**Merck Index Number** 9727

### Chemical Structure



## T

**Chemical/Dye Class** Nitro

**Molecular Formula**  $C_7H_3N_3O_8$

**Molecular Weight** 257.11

**pH Range** 12.0–13.4

**Color Change at pH** Colorless (12.0) to orange (13.4)

**pKa** 0.42, 0.65

**Physical Form** Light yellow crystals

**Solubility** Solubler in water, ethanol, methanol, ether, acetone

**Melting Point** 228.7°C

**Boiling Point (Calcd.)**  $435.8 \pm 45.0^\circ\text{C}$  Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–6</sup>

**Applications** Explosive,<sup>7–11</sup> liquefied gas fuels,<sup>12,13</sup> energetic materials,<sup>14</sup> antiwear agent,<sup>15,16</sup> electroconductive polymers,<sup>17,18</sup> photography,<sup>19,20</sup> photoconductor,<sup>21</sup> recording materials,<sup>22</sup> inks,<sup>23</sup> adhesives<sup>24</sup>

**Safety/Toxicity** Genotoxicity,<sup>25</sup> mutagenicity,<sup>26</sup> chemical toxicity to aquatic organisms<sup>27</sup>

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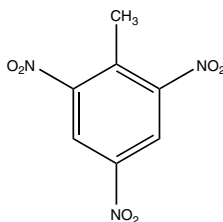
## TRINITROTOLUENE

**Other Names** Toluene, 2,4,6-trinitro-;  $\alpha$ -TNT; 1-Methyl-2,4,6-trinitrobenzene; 2,4,6-Trinitrotoluene; 2-Methyl-1,3,5-trinitrobenzene; 4-Methyl-1,3,5-trinitrobenzene; Gradetol; NSC 36949; TNT; Tolit; Tolite; Trinitrotoluene; Tritol; Tritol (explosive); Trotyl; Trotyl oil; sym-Trinitrotoluene; sym-Trinitrotoluol

**CA Index Name** Benzene, 2-methyl-1,3,5-trinitro-

**CAS Registry Number** 118-96-7

**Merck Index Number** 9730

**Chemical Structure**

**Chemical/Dye Class** Nitro

**Molecular Formula** C<sub>7</sub>H<sub>5</sub>N<sub>3</sub>O<sub>6</sub>

**Molecular Weight** 227.13

**pH Range** 11.5–14.0

**Color Change at pH** Colorless (11.5) to orange (14.0)

**Physical Form** Yellow crystals

**Solubility** Very sparingly soluble in water; soluble in acetone, benzene; less soluble in ethanol

**Melting Point** 80.1°C

**Boiling Point** 335–340°C

**Synthesis** Synthetic methods<sup>1–7</sup>

**Major Applications** Explosive,<sup>3,7–10</sup> energetic materials,<sup>11,12</sup> preparation of diamond<sup>13–15</sup>

**Safety/Toxicity** Ecotoxicity,<sup>16</sup> genotoxicity,<sup>17</sup> cytotoxicity,<sup>18</sup> oral toxicity,<sup>19</sup> phytotoxicity,<sup>20</sup> human toxicological effect,<sup>21</sup> environmental pollutants,<sup>22</sup> soil toxicity,<sup>23</sup> mutagenicity<sup>24</sup>

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## TROPAEOLIN O

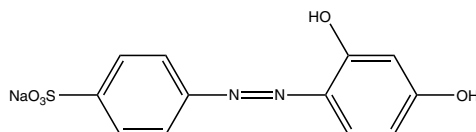
**Other Names** C.I. Acid Orange 6; C.I. Acid Orange 6, monosodium salt; Chrysoin S; Benzenesulfonic acid, *p*-(2,4-dihydroxyphenylazo)-, sodium salt; 2,4-Dihydroxyazobenzene-4'-sulfonate sodium salt; Acid Leather Yellow PGW; Acid Orange 6; Acid Phosphine G New; Acme Yellow Acid Yellow RS; C Yellow 12; C.I. 14270; C.I. Food Yellow 8; Cetil Chromine Yellow GR; Chrysoin G; Chrysoin S Specially Pure; Chrysoine; Chrysoine Extra; Chrysoine Extra Pure A; Chrysoine N; Chrysoine S; Chrysoine S Extra Pure; Chrysonine S; Curol Orange G; Dermina Yellow G; E 103; E 103 (dye); Eniacid Yellow RS; Eurocert Chrysoine S; Gold yellow; Hispacid Yellow CG; Naphthazine Yellow RP; Neklacid Yellow G; Orange Acid G; Orange VI; Resorcin yellow; Resorcine Yellow; Resorcine Yellow O Extra; Resorcinol Yellow A; Resorcinol yellow; Sodium azoresorcinolsulfanilate; Tertracid Yellow TRO; Tropaeolin O; Tropaeolin R; Tropaeoline; Tropeolin O; Yellow T

**CA Index Name** Benzenesulfonic acid, 4-[(2,4-dihydroxyphenyl)azo]-, monosodium salt

**CAS Registry Number** 547-57-9

**Merck Index Number** 9775

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{12}H_9N_2NaO_5S$

**Molecular Weight** 316.27

**pH Range** 11.0–12.7

**Color Change at pH** Yellow (11.0) to red (12.7)

**pKa** 11.5, 11.9

**Physical Form** Orange-red powder

**Solubility** Soluble in water, ethanol

**UV-Visible ( $\lambda_{max}$ )** 490 nm

**Melting Point** >300°C

**Synthesis** Synthetic methods<sup>1–3</sup>

**Major Applications** Photoresists,<sup>4</sup> image forming materials,<sup>5</sup> nonlinear optical (NLO) materials,<sup>6</sup> silicon etching,<sup>7</sup> photography,<sup>8</sup> inks,<sup>9</sup> markers,<sup>10</sup> lithium battery,<sup>11</sup> leather dyes,<sup>12</sup> polishing stainless steel,<sup>13</sup> concrete,<sup>14,15</sup> automobile radiators,<sup>16</sup> textiles,<sup>17,18</sup> cleaners,<sup>19</sup> hair dyes,<sup>20–23</sup> food storage,<sup>24</sup> cosmetics,<sup>25–29</sup> immunomodulating agents,<sup>30</sup> disinfectant,<sup>31</sup> antihistaminic agent,<sup>32</sup> antimicrobial agent,<sup>33</sup> nucleic acids<sup>34</sup>

**Safety/Toxicity** Toxic quantitative structure-activity relationships,<sup>35</sup> toxicity to aquatic microbial populations,<sup>36</sup> genotoxicity<sup>37</sup>

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## TROPAEOLIN OO

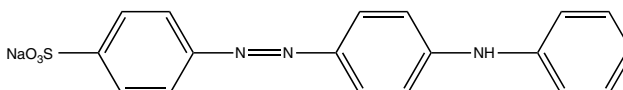
**Other Names** Benzenesulfonic acid, *p*-(*p*-anilinophenylazo)-, sodium salt; C.I. Acid Orange 5; C.I. Acid Orange 5, monosodium salt; Acid Orange 5; Acid Orange IV; Acid Yellow D; Aniline Yellow; C.I. 13080; Diphenylamine Orange; Hispacid Orange IV; Orange GS; Orange IV; Orange N; Solar Orange IV; Tertracid Orange IV; Tropaeolin OO; Tropeolin OO

**CA Index Name** Benzenesulfonic acid, 4-[[4-(phenylamino)phenyl]azo]-, monosodium salt

**CAS Registry Number** 554-73-4

**Merck Index Number** 9776

### Chemical Structure



**Chemical/Dye Class** Azo

**Molecular Formula** C<sub>18</sub>H<sub>14</sub>N<sub>3</sub>O<sub>3</sub>SNa

**Molecular Weight** 375.38

**pH Range** 1.4–2.6

**Color Change at pH** Red (1.4) to yellow (2.6)

**pKa** 2.0

**Physical Form** Orange-yellow powder

**Solubility** Soluble in water, ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 527 nm

**Melting Point** >300°C

**Synthesis** Synthetic methods<sup>1–4</sup>

**Major Applications** Sensors,<sup>5</sup> lithographic plates,<sup>6</sup> optical recording media,<sup>7</sup> photoreceptor,<sup>8</sup> inks,<sup>9</sup> indication system for product exceeding threshold temperature,<sup>10</sup> lubricants,<sup>11</sup> textiles,<sup>12</sup> food storage,<sup>13</sup> determination of amiodarone,<sup>14</sup> astemizole,<sup>15</sup> bromhexine,<sup>16</sup> clomipramine,<sup>17</sup> deutiforin,<sup>18</sup> domperidone,<sup>19</sup> fluoroquinolone,<sup>20</sup> roxithromycin,<sup>21</sup> terfenadine,<sup>22</sup> thiabendazole,<sup>23</sup> antihistamines<sup>24</sup>

**Safety/Toxicity** Biodegradation and toxicity<sup>25</sup>

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## TROPAEOLIN OOO

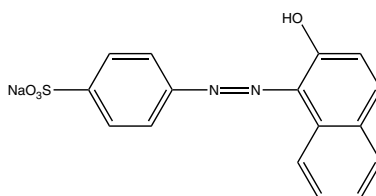
**Other Names** Acid Orange; Acid Orange A; C.I. Acid Orange 7, monosodium salt; Benzenesulfonic acid, *p*-(2-hydroxy-1-naphthylazo)-, sodium salt;  $\beta$ -Naphthol Orange;  $\beta$ -Naphthyl orange; 11550 Orange; 2-Naphthol Orange II; AO 7; Acid Leather Orange PRW; Acid Leather Orange extra; Acid Orange 7; Acid Orange II; Acilan Orange II; Airedale Orange II; Amacid Orange Y; Amacid Orange Y Conc; Atul Acid Orange II; Basacid Orange 280; Basacid Orange 282; Betanaphthol orange; Brasilan Orange A; Bucacid Orange A; C Ext. Orange 8; C.I. 15510; C.I. Acid Orange 7; Calcocid Orange Y; Certiquel Orange II; Colacid Orange; Curol Orange; D and C Orange No. 4; D&C Orange #4; D&C Orange No. 4; Diacid Orange II; Duasyn Acid Orange P; Egacid Orange II; Erio Orange II; Everacid Orange II; Fenazo Orange; Hidacid Orange II; Hispacid Orange AF; Japan Orange 205; Japan Orange No. 205; Java Orange II; Keyacid Orange II; Kiton Orange II; Kromon Lake Orange Toner; Lake Orange A; Lake Orange II YS; Leather Orange Extra; Lurazol Orange E; Lurazol Orange EBR; Lutetia Orange 3JR; Mandarin G; Naphthalene Lake Orange G; Naphthalene Orange G; Naphthol Orange; Naphthocard Orange II; Neklacid Orange II; No. 177 Orange Lake; Nubilon Orange R; Orange 2; Orange 2 sodium salt; Orange Extra N; Orange Extra P; Orange II; Orange II Special For Lacquer; Orange II for Lakes; Orange IIC; Orange IIP; Orange IIS; Orange IISM; Orange No. 205; Orange Toner GRT; Orange Y; Orange YA; Orange YZ; Peer-acid Orange II; Persian Orange; Persian Orange Lake; Persian Orange X; Pure Orange II S; Rifa Acid Orange II; Rybacel Orange A; Sanyo Gum Orange A; Sodium 4-(2-hydroxy-1-naphthylazo)benzenesulfonate; Solar Orange; Special Orange GR; Special Orange H; Symuler Orange Lake 43; Symulon Acid Orange II; Takaoka Acid Orange II; Tangarine Lake X 917; Tertracid Orange II; Tropaeolin OOO; Tropaeolin OOO 2; Tropeolin OOO; Vondacid Orange II; Wool Orange A; *p*-(2-Hydroxy-1-naphthylazo)benzenesulfonic acid sodium salt

**CA Index Name** Benzenesulfonic acid, 4-[(2-hydroxy-1-naphthalenyl)azo]-, monosodium salt

**CAS Registry Number** 633-96-5

**Merck Index Number** 6858

**Chemical Structure**



**Chemical/Dye Class** Azo

**Molecular Formula**  $C_{16}H_{11}N_2O_4SNa$

**Molecular Weight** 350.33

**pH Range** 7.4–8.6;

10.2–11.8

**Color Change at pH** Amber (7.4) to orange (8.6)

Orange (10.2) to red (11.8)

**pKa** 8.26, 11.4

**Physical Form** Orange-brown powder

**Solubility** Very soluble in water; very slightly soluble in ethanol

**UV-Visible ( $\lambda_{max}$ )** 483 nm

**Melting Point** >300°C

**Synthesis** Synthetic methods<sup>1–6</sup>

**Major Applications** Organic light emitting diodes (OLEDs),<sup>7</sup> nanoparticles,<sup>8</sup> inks,<sup>9</sup> wood preservatives,<sup>10</sup> textiles,<sup>11</sup> hair dyes,<sup>12,13</sup> cosmetics,<sup>14,15</sup> wound dressing materials,<sup>16</sup> biofuel cells<sup>17</sup>

**Safety/Toxicity** Acute toxicity,<sup>18</sup> carcinogenicity,<sup>19</sup> genotoxicity,<sup>20</sup> toxicity to fish,<sup>21</sup> mutagenicity<sup>22,23</sup>

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# U

## UMBELLIFERONE

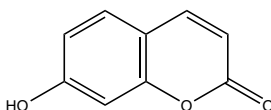
**Other Names** Coumarin, 7-hydroxy-; 7-Hydroxy-2-chromenone; 7-Hydroxy-2H-1-benzopyran-2-one; 7-Hydroxy-2H-chromen-2-one; 7-Hydroxycoumarin; 7-Oxycoumarin; Hydrangin; Hydrangine; NSC 19790; Skimmetin; Skimmetine; Umbelliferon; Umbelliferone

**CA Index Name** 2H-1-Benzopyran-2-one, 7-hydroxy-

**CAS Registry Number** 93-35-6

**Merck Index Number** 9847

**Chemical Structure**



**Chemical/Dye Class** Fluorescent, Coumarin

**Molecular Formula** C<sub>9</sub>H<sub>6</sub>O<sub>3</sub>

**Molecular Weight** 162.14

**pH Range** 6.5–8.0

**Color Change at pH** Nonfluorescence (6.5) to blue fluorescence (8.0)

**pKa** 7.11

**Physical Form** Off-white to tan powder

**Solubility** Slightly soluble in boiling water; freely soluble in ethanol, chloroform, acetic acid

**UV-Visible ( $\lambda_{\text{max}}$ )** 320 nm

**Melting Point** 225–228°C

**Boiling Point (Calcd.)** 382.1 ± 37.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–6</sup>

**Major Applications** Fluorescent brighteners,<sup>7</sup> fungicides,<sup>8</sup> cosmetics,<sup>9</sup> antitrypanosomal,<sup>10</sup> anti-leishmanial activities,<sup>10</sup> antifungal,<sup>11</sup> antibacterial,<sup>11</sup> Antiinflammatory,<sup>12</sup> antiHIV,<sup>13</sup> detection of microorganisms,<sup>14</sup> treatment of impaired neurotransmission disorders,<sup>15</sup> Alzheimer's disease,<sup>16</sup> vascular and lymphatic edema<sup>17</sup> cancer,<sup>18</sup> early diagnosis of stroke,<sup>19</sup> dental material,<sup>20</sup> drug-coated coronary stent system<sup>21</sup>

**Safety/Toxicity** Acute oral toxicity,<sup>22</sup> cytotoxicity,<sup>23</sup> mutagenicity<sup>24</sup>

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# X

## XYLENOL BLUE

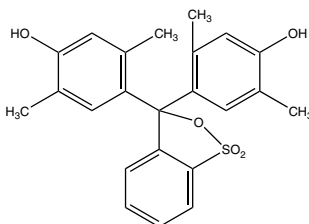
**Other Names** 2,5-Xylenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)di-, *S,S*-dioxide; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)*bis*[2,5-dimethyl-, *S,S*-dioxide; *p*-Xylenolsulfonephthalein; *p*-Xylenolsulfophthalein; 3H-2,1-Benzoxathiole, phenol derivative; 1,4-Dimethyl-5-hydroxybenzenesulfonphthalein; NSC 10471; Xylenol blue; *p*-Xylenesulfonephthalein; *p*-Xylenol blue; *p*-Xylenolsulfonphthalein

**CA Index Name** Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*[2,5-dimethyl-

**CAS Registry Number** 125-31-5

**Merck Index Number** 10083

**Chemical Structure**



**Chemical/Dye Class** Sulfonephthalein

**Molecular Formula** C<sub>23</sub>H<sub>22</sub>O<sub>5</sub>S

**Molecular Weight** 410.48

**pH Range** 1.2–2.8;

8.0–9.6

**Color Change at pH** Red (1.2) to yellow (2.8)

Yellow (8.0) to blue (9.6)

**pKa** 9.52

**Physical Form** Dark brown powder

**Solubility** Slightly soluble in water, soluble in ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 424 nm

**Melting Point** 212°C (decompose)

**Boiling Point (Calcd.)** 577.2 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Electrochromic displays,<sup>6</sup> chemical sensors,<sup>7</sup> fiber-optic pH sensors,<sup>8</sup> optical-quality films,<sup>9</sup> ink,<sup>10</sup> corrosion testing,<sup>11</sup> lubricants,<sup>12</sup> TTI indicators,<sup>13</sup> food storage,<sup>14</sup> cosmetics,<sup>15</sup> determining bacterial growth,<sup>16</sup> microbiological assays,<sup>17</sup> determining lipase,<sup>18</sup> drugs<sup>19</sup>

**Safety/Toxicity** Mutagenicity<sup>20</sup>

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## XYLENOL ORANGE

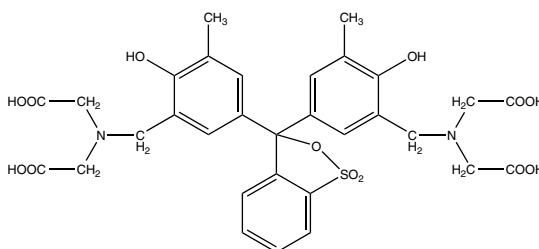
**Other Names** Acetic acid, [( $\alpha$ -hydroxy-*o*-sulfobenzylidene)bis[(6-hydroxy-5-methyl-*m*-phenylene)methylenenitrilo]]tetra-,  $\gamma$ -sultone; Acetic acid, [3H-2,1-benzoxathiol-3-ylidenebis[(6-hydroxy-5-methyl-*m*-phenylene)methylenenitrilo]]tetra-, *S,S*-dioxide; Glycine, *N,N'*-[3H-2,1-benzoxathiol-3-ylidenebis[(6-hydroxy-5-methyl-3,1-phenylene)methylene]]bis[*N*-(carboxymethyl)-, *S,S*-dioxide; Phenolsulfonephthalein, 3',3''-bis[[bis(carboxymethyl)amino]-methyl]-5',5''-dimethyl-, 3H-2,1-Benzoxathiole, glycine derivative; Cresol Phthalexon S; NSC 324982; Xylenol Orange; *o*-Cresolphthalexon S

**CA Index Name** Glycine, *N,N'*-[[(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[(6-hydroxy-5-methyl-3,1-phenylene)methylene]]bis[*N*-(carboxymethyl)-

**CAS Registry Number** 1611-35-4

**Merck Index Number** Not listed

### Chemical Structure



**Chemical/Dye Class** Sulfonphthalein

**Molecular Formula** C<sub>31</sub>H<sub>32</sub>N<sub>2</sub>O<sub>13</sub>S

**Molecular Weight** 672.66

**pH Range** 6.4–10.4

**Color Change at pH** Yellow (6.4) to orange-red (10.4)

**pKa** 2.6, 6.4, 6.5, 10.5, 12.3

**Physical Form** Brown powder

**Solubility** Soluble in water, ethanol

**UV-Visible** ( $\lambda_{\text{max}}$ ) 580 nm

**Melting Point** 210°C (decompose)

**Boiling Point (Calcd.)** 895.1  $\pm$  65.0°C Pressure: 760

**Synthesis** Synthetic methods<sup>1–5</sup>

**Major Applications** Solar cells,<sup>6</sup> cosmetics,<sup>7</sup> determination of aluminum,<sup>8</sup> nickel,<sup>8</sup> bismuth,<sup>9</sup> thallium,<sup>10</sup> lead,<sup>11</sup> zinc,<sup>11</sup> palladium,<sup>12</sup> mercury,<sup>13</sup> proteins,<sup>14</sup> lipids<sup>15</sup>

**Safety/Toxicity** Carcinogenicity<sup>16</sup>

### References

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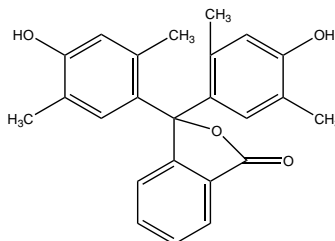
## XYLENOLPHTHALEIN

**Other Names** *p*-Xylenolphthalein, 2',5',2'',5''-tetramethylphenolphthalein

**CA Index Name** 1(3H)-Isobenzofuranone, 3,3-*bis*(4-hydroxy-2,5-dimethylphenyl)-

**CAS Registry Number** 50984-88-8

**Merck Index Number** Not listed

**Chemical Structure**

**Chemical/Dye Class** Phthalein

**Molecular Formula** C<sub>24</sub>H<sub>22</sub>O<sub>4</sub>

**Molecular Weight** 374.43

**pH Range** 9.0–10.5

**Color Change at pH** Colorless (9.0) to indigo-blue (10.5)

**pKa** 9.7

**Physical Form** Pale yellow or cream-colored powder

**Solubility** Insoluble in water; soluble in ethanol, acetone

**Melting Point** 276°C

**Boiling Point (Calcd.)** 569.6 ± 50.0°C Pressure: 760 Torr

**Synthesis** Synthetic methods<sup>1,2</sup>

**Major Applications** Inks,<sup>3,4</sup> detergent,<sup>5</sup> photoresist,<sup>6,7</sup> toothpaste and mouthwash,<sup>8</sup> disinfectant,<sup>9</sup> cosmetics,<sup>10</sup> paints<sup>11</sup>

**Safety/Toxicity** No data available

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# HANDBOOK OF ACID-BASE INDICATORS

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