

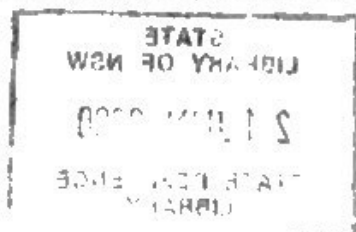
THE
MERCK
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★
TWELFTH EDITION

THE MERCK INDEX

AN ENCYCLOPEDIA OF
CHEMICALS, DRUGS, AND BIOLOGICALS

TWELFTH EDITION

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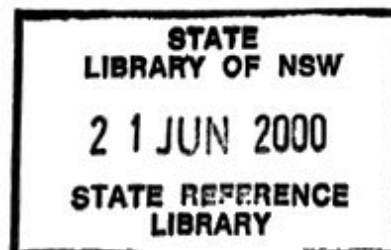
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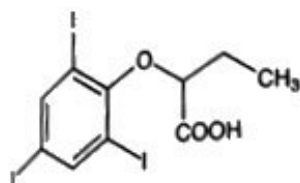


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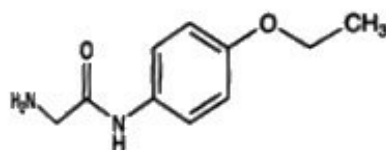
(3 different phases), mp 174-178°. uv max (pH
40 nm ($A_{1\text{cm}}^{1\%}$) 431). (0.1N NaOH): 256 nm ($A_{1\text{cm}}^{1\%}$)
Slightly better taste. One gram dissolves in about one
water. 8 ml alc. 40 ml chloroform, 13 ml ether,
no ml benzene. Soluble in alkali hydroxides and
A satd aq soln is acid to litmus. pK_1 7.3, pK_2
orally in rats: 162 ± 14 mg/kg (Goldenthal).
 $C_{12}H_{11}N_2NaO_3$, sol phenobarbital, sol pheno-
bitter, slightly hygroscopic crystals or white
One gram dissolves in about 1 ml water, about 10
Insol in ether or chloroform. Aq solns are
litmus and phenolphthalein, pH ~9.3. LD₅₀
660 mg/kg (Schaffarick, Brown).
May be habit forming. This is a controlled
(depressant) listed in the U.S. Code of Federal
Title 21 Parts 329.1 and 1308.14 (1995).
Anticonvulsant; sedative; hypnotic.
AT VET: Anticonvulsant; sedative.

Phenobutidil. 2-(2,4,6-Triiodophenoxy)butanoic
acid; 1-(2,4,6-triiodophenoxy)propanecarb-
onic acid; 1-(2,4,6-triiodophenoxy)butyric acid; α-(2,4,6-triiodo-
phenoxy)butyric acid. C₁₀H₉I₃O₃; Baynostil; Vésipaque. C 21 53%, H 1.63%, I 68.24%, O 8.60%.
Rudel et al., Bull. Soc. Chim. France 1954, 342;
U.S. pat. 2,796,432 (1957 to Chimie et
Pharmacology: H. Bekker et al., Pharmazie



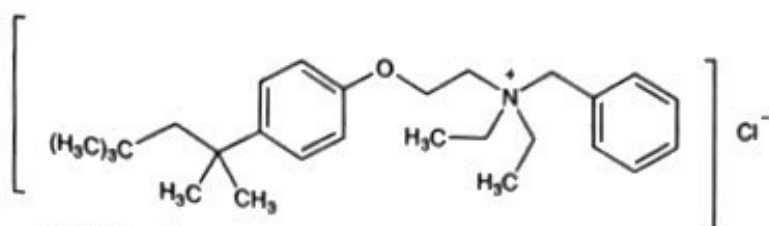
Diagnosis: aid (radiopaque medium—chole-

Phenocoll. 2-Amino-N-(4-ethoxyphenyl)acetamide; α-amino-p-acetophenetidine; 4-glycylaminophenol ethyl ester; p-acetophenetidine; 4-glycylaminophenetol; glycylamidoacetic acid phenol salt; Phenamine. C₁₀H₁₄N₂O₃; mol wt 226.27. C 61.84%, H 7.27%, N 14.42%, O 16.47%. Ger. pat. 59,121; 59,874 (1891 to Schering); U.S. pat. 2,915,918; Ger. pat. 346,809 (1921 to Schering), U.S. 1,066, Karrer, Haebler, Helv. Chim. Acta 7, 534 (1924).



anhydrous, mp 100.5°.
 dihydrate, crystals, mp 95°.
 hydrochloride, $C_{10}H_{14}N_2O_2 \cdot HCl$, cryst powder. Sol in 20
 parts water, in alcohol. More sol in hot water; slightly sol
 in benzene, chloroform, ether. Aq soln is neutral. *Incom-*
patible with alkali hydroxides or carbonates.
 acetate, $C_{10}H_{14}N_2O_2 \cdot C_2H_3O_2$, *Salocoll*. Fine needles.
 Sweet taste. Sol in 200 parts cold, 20 parts hot water.
 As for the hydrochloride; with substances in-
 compatible with salicylates.
 CAT Antipyretic, analgesic.

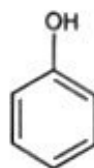
Phenoxide, *N,N*-Diethyl-*N*-{2-[4-(1,1,3,3-tetra-
methylphenoxy)ethyl]benzenemethanaminium chloride;
2-(*p*-1,1,3,3-tetramethylbutyl)phenoxyethylam-
monium chloride; *β*-*p*-tert-octylphenoxyethyl-diethylbenzyl-
ammonium chloride; Octaphen. $C_{27}H_{44}ClNO$; mol wt
376.7. C 75.09%, H 9.80%, Cl 8.20%, N 3.24%, O 3.70%.
Goldberg, Besly, Brit. pat. 703,477 (1954 to Ward
& Co., London). Erekaev, *C.A.* 54, 12483i (1960).



Crystals from ethyl acetate. mp 112-114° (Goldberg, Besly); mp 95° (Erekaev).

USE: Orthophosphate as lubricant: Semmens, Summers-Smith, Brit. pat. 790,056 (1958 to I.C.I.).
THERAP CAT: Anti-infective (topical).

7390. Phenol. Carboic acid; phenic acid; phenylic acid; phenyl hydroxide; hydroxybenzene; oxybenzene. C_6H_5O ; mol wt 94.11. C 76.57%, H 6.43%, O 17.00%. Obtained from coal tar, or made by fusing sodium benzene-sulfonate with NaOH, or by heating monochlorobenzene with aq NaOH under high pressure. The crystalline article of commerce contains at least 98% phenol. Review of mfg processes: A. Dierichs, R. Kubicka, *Phenole und Basen. Vorkommen und Gewinnung* (Akademie-Verlag, Berlin, 1958) 472 pp; Faith, Keyes & Clark's *Industrial Chemicals*, F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 612-623. Use in treatment of spasticity: D. E. Garland *et al.*, *Clin. Orthop.* **165**, 217 (1982); *idem*, *Arch. Phys. Med. Rehab.* **65**, 243 (1984). Review of use in pain relief: K. M. Wood, *Pain* **5**, 205-229 (1978). Review of toxicology: H. Babich, D. L. Davis, *Regul. Toxicol. Pharmacol.* **1**, 90-109 (1981). Toxicity: W. B. Deichmann, S. Witherup, *J. Pharmacol. Exp. Ther.* **80**, 233 (1944). Review: C. Thurman in *Kirk-Othmer Encyclopedia of Chemical Technology* vol. 17 (Wiley-Interscience, New York, 3rd ed., 1982) pp 373-384.



Colorless, acicular crystals or white, crystalline mass. Characteristic odor, somewhat sickeningly sweet and acrid with a sharp and burning taste. *Poisonous and caustic!* Prone to redden on exposure to air and light, hastened by presence of alkalinity. d 1.071. When free from water and cresols it congeals at 41° and melts at 43°. Ultrapure material mp 40.85°. The commercial product contains an impurity which raises the mp. bp 182°. Flash pt, closed cup: 175°F (79°C). n_D^{20} 1.5425. pKa at 25° = 10.0. pH of aq solns ~6.0. It is liquefied by mixing with ~8% water. One gram dissolves in ~15 ml water, 12 ml benzene; very sol in alcohol, chloroform, ether, glycerol, carbon disulfide, petrolatum, volatile and fixed oils, aq alkali hydroxides. Almost insol in petr ether. LD₅₀ orally in rats: 530 mg/kg (Deichmann, Witherup). *Keep well closed and protected from light. Do not handle with bare hands.*

Ammonium salt, $C_6H_6O.NH_3$, *ammonium phenate*, *ammonium carbolate*. White to pink crystalline masses. Sol in water.

Sodium salt, C_6H_5NaO , *phenolate sodium*.

Aqueous solution with phenolate sodium, *Chloraseptic*.

Cautions: Phenol is rapidly absorbed through skin, and from the stomach and lungs. Systemic toxicity can result from ingestion of solutions, or from inhalation or cutaneous absorption of solutions or vapor. This is characterized by an initial excitatory phase, rapidly progressing to fulminating CNS depression with coma. Potential symptoms of acute overexposure are stearorous breathing, mucous rales, froth at mouth and nose, frank pulmonary edema; cyanosis; tremor, convulsions, twitching; death due to respiratory failure. Characteristic odor of phenol on breath. Ingestion may cause burning of mouth and throat; white necrotic lesions in mouth, esophagus and stomach; abdominal pain. Direct contact may cause irritation of eyes, nose and throat; skin burns; dermatitis; ochronosis. Chronic exposure may result in vomiting, difficulty swallowing, excess salivation, diarrhea, anorexia, weight loss; headache, fainting, vertigo.

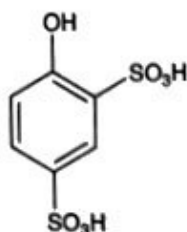
mental disturbances; muscle aches and pain, weakness; damage to liver and kidney, dark urine. See *NIOSH Pocket Guide to Chemical Hazards* (DHHS/NIOSH 90-117, 1990) p 176; *Clinical Toxicology of Commercial Products*, R. E. Gosselin et al., Eds. (Williams & Wilkins, Baltimore, 5th ed., 1984) Section III, p344-348; *Patty's Industrial Hygiene and Toxicology* vol. 2A, G. D. Clayton, F. E. Clayton, Eds. (Wiley-Interscience, New York, 3rd ed., 1981) p 2567-2584.

USE: As a general disinfectant, either in soln or mixed with slaked lime, etc., for toilets, stables, cesspools, floors, drains, etc.; for the manuf of colorless or light-colored artificial resins, many medical and industrial organic compds and dyes; as a reagent in chemical analysis. Pharmaceutical aid (preservative).

THERAP CAT: Aqueous soln as topical anesthetic; topical antiseptic; topical antipruritic.

THERAP CAT (VET): Antiseptic caustic. Topical anesthetic in pruritic skin conditions. Has been used internally and externally as an antiseptic.

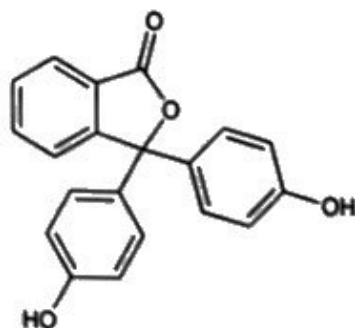
7391. Phenoldisulfonic Acid. 4-Hydroxy-1,3-benzenedisulfonic acid; 4-hydroxy-m-benzenedisulfonic acid; 1-phenol-2,4-disulfonic acid. $C_6H_6O_5S_2$; mol wt 254.24. C 28.35%, H 2.38%, O 44.05%, S 25.22%. Conveniently prep'd by hydrolysis of the dichloride which is obtained by the action of chlorosulfonic acid on phenol at room temp: Pollak et al. *Monatsh.* 46, 395 (1925). Monograph: E. E. Gilbert, *Sulfonation and Related Reactions* (Interscience, New York, 1965) 529 pp.



Deliquescent needles, vague melting range from 89° to 100°. Decomp above 100°. Freely sol in water, methanol. Practically insol in ether, petr ether.

USE: In the manuf of aminophenoldisulfonic acids which are intermediates in the dye industry.

7392. Phenolphthalein. 3,3-Bis(4-hydroxyphenyl)-1-(3H)-isobenzofuranone; 3,3-bis(p-hydroxyphenyl)phthalide; α -(p-hydroxyphenyl)- α -(4-oxo-2,5-cyclohexadien-1-ylidene)-o-toluic acid; Choclox; Darmol. $C_{20}H_{14}O_4$; mol wt 318.33. C 75.46%, H 4.43%, O 20.10%. Prep'd by condensing phenol with phthalic anhydride: Baeyer, *Ann.* 202, 69 (1880); Herzog, *Chem. Ztg.* 51, 84 (1927); Hubacher, U.S. pat. 2,192,485 (1940 to Ex Lax); Gamrath, U.S. pat. 2,522,939 (1950 to Monsanto). Subchronic toxicity studies: D. D. Dietz et al., *Fund. Appl. Toxicol.* 18, 48 (1992). Comprehensive description: F. J. Al-Shammery et al. in *Analytical Profiles of Drug Substances* vol. 20, K. Florey Ed. (Academic Press, New York, 1991) pp 627-664.



Minute, triclinic crystals, often twinned. mp 258-262°. d 1.299. Color: White or yellowish-white. see also Yellow Phenolphthalein. Sol in alcohol and ether, very slightly sol in chloroform. One gram dissolves in 12 ml alcohol, in ~100 ml ether. Almost insol in water. Sol in dil solns of alkali hydroxides and hot solns of alkali carbonates forming a red soln. pKa (25°C) 9.7. uv max (methanol): 205, 229, 276 nm (ϵ 27261.147, 14692.144, 2006.369).

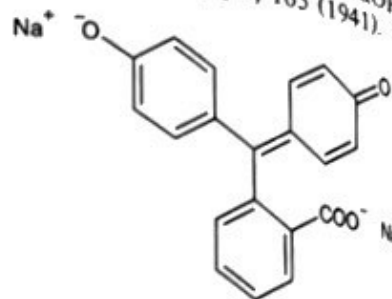
USE: A 1% alcoholic soln as an indicator in titrations of mineral and organic acids and most alkalies. Not suitable

for ammonia. Very sensitive to CO_2 and in carbonates the liq must be boiled. Borax can be present, because the color gradually fades away as the pink to deep-red, > pH 9.

THERAP CAT: Cathartic.

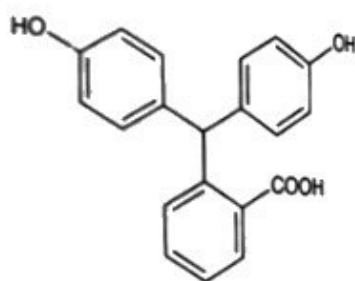
THERAP CAT (VET): Has been used as a laxative.

7393. Phenolphthalein Sodium. 3,3-Bis(4-hydroxyphenyl)-1-(3H)-isobenzofuranone disodium salt. $C_{20}H_{12}O_4Na_2$; mol wt 362.29. C 66.31%, H 3.34%, Na 17.66%. Prep'd from an alcoholic soln of 1 mol phthalein by the addition of 2 mols NaOH (12.6 g). Buu-Hoi, *Bull. Soc. Chim.* [5] 8, 165 (1941).



Reddish-brown granular mass with coppery luster; pale red powder. Dec in air. Soluble in water, green, deep-red soln. Absorption max: 550-555 nm. The enol form is colorless, as is the trisodium salt.

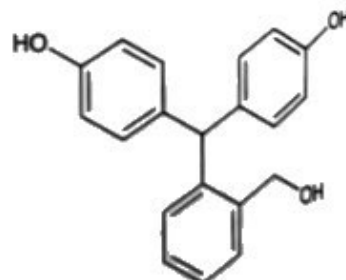
7394. Phenolphthalin. 2-[Bis(4-hydroxyphenyl)methoxy]benzoic acid; decolorized phenolphthalein. phthalin. 4,4'-dihydroxytriphenylmethane-2-carboxylic acid. $C_{20}H_{14}O_5$; mol wt 320.34. C 74.99%, H 5.03%, O 19.98%. Made by boiling phenolphthalein with zinc dust in alkaline soln. Called "Kastle-Meyer reagent" when in soln. Prep'd by dissolving 2 g phenolphthalin + 20 g KOH in a desired amount of doubly distd H_2O and diluting with an equal vol of ethanol. Detailed directions for prep'n of test soln and use: Lecoq, *Bull. Soc. Chim. Belge* 54, 186-202 (1945). *CA* 41, 2346i (1947).



Colorless crystals, mp 237°. Insol in water; sol in alcohol, ether, aq alkali. The alkaline solns gradually become brown on exposure to air or other oxidizing substances.

USE: As a reagent for oxidases, blood, HCN, peroxide, copper.

7395. Phenolphthalol. 2-[Bis(4-hydroxyphenyl)methoxy]benzenemethanol; o-[bis(p-hydroxyphenyl)methoxy]benzyl alcohol; dihydroxyphenylmethenylbenzyl alcohol; bis(4-hydroxyphenyl)methenylbenzyl alcohol; bis(4-hydroxyphenyl)methane-2-hydroxymethylphenylmethane; Egmol; Regolax. $C_{20}H_{18}O_5$; mol wt 306.36. C 78.41%, H 5.92%, O 15.67%. Prep'n: Hubacher, *J. Am. Chem. Soc.* 74, 5216 (1952). Schultz, Geller, *Arch. Pharm.* 288, 234 (1955). *Bull. Soc. Chim. Belge* 59, 1538 (1946). *CA* 59, 1538 (1946).



Crystals from dil alcohol, mp 201-202°.

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