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THIRTEENTH EDITION

# THE MERCCK INDEX

AN ENCYCLOPEDIA OF  
CHEMICALS, DRUGS, AND BIOLOGICALS

THIRTEENTH EDITION

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*Published by*  
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**MERCK & CO., INC.**  
Whitehouse Station, NJ

2001

EDITION

**MERCK & CO., INC.**  
Whitehouse Station, NJ  
USA

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1st Edition—1889  
2nd Edition—1896  
3rd Edition—1907  
4th Edition—1930  
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7th Edition—1960  
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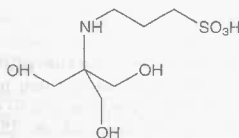
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Library of Congress Catalog  
Card Number 89-60001  
ISBN Number 0911910-13-1

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**9148. TAPS.** [29915-38-6] 3-[[2-Hydroxy-1,1-bis(hydroxymethyl)ethyl]amino]-1-propanesulfonic acid; *N*-tris(hydroxymethyl)ethylamino]-1-propanesulfonic acid.  $C_7H_{17}NO_5S$ ; mol wt 243.28. C 34.56%, H 7.04%, N 5.76%, O 46.64%. S 13.18%. Zwitterionic *N*-substituted sulfonic acid in the style of the "Good" buffers; active in the pH range 6-8.5. Prepn: I. Zeid, I. Ismail, *Ann.* **1974**, 667. Dissociation: A. M. El-Naby, H. A. Azab, *Acta Chim. Hung.* **130**, 665 (1993). Use as eluent: R. H. P. Reid, *J. Chromatog. A* **684**, 221 (1994). Effect of buffer concentration on pH-activity relationship: C. G. Bevans, A. L. Harris, *J. Biol. Chem.* **274**, 3711 (1999).



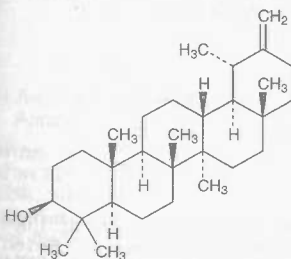
Crystals, mp 194°. pKa: 8.55; pKa (37°): 8.1; pKa<sub>2</sub> (25°): 8.25.

**TAPSO.** [68399-81-5] 2-Hydroxy-3-[[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]amino]-1-propanesulfonic acid.  $C_7H_{17}NO_5S$ ; mol wt 259.28. Hydroxy analog of TAPS. Prepn: W. I. Ferguson *et al.*, *Anal. Biochem.* **104**, 300 (1980). Crystal structure: J. Wouters, D. Stalke, *Acta Crystallog.* **C52**, 1684 (1996). Thermodynamics of dissociation: R. N. Roy *et al.*, *J. Chem. Eng. Data* **42**, 446 (1997). Triclinic colorless crystals, mp 226-228° (dec). pKa (20°): 7.7.  $\Delta pK_a/C$ : -0.018. Soly in water (0°): 1M.

USE: Biological buffer.

**9149. Taraxacum.** Dandelion; lion's tooth. Dried rhizome and roots of *Taraxacum palustre* (Lyons) Lam. & DC. (*T. officinale* Weber, *Leontodon taraxacum* L.), *Compositae*. *Habit* Europe; naturalized in North America. *Constit.* Taraxantholone, levulin, inulin, pectin.

**9150. Taraxasterol.** [1059-14-9] (3 $\beta$ ,18 $\alpha$ ,19 $\alpha$ )-Urs-20(30)-en-3-ol; taraxast-20(30)-en-3 $\beta$ -ol; anthesterin;  $\alpha$ -lactucerol; taraxasterin.  $C_{30}H_{50}O$ ; mol wt 426.72. C 84.44%, H 11.81%, O 1.75%. A monohydroxy triterpene. Isolated from *Taraxacum officinale*. Wiggers, *Compositae*: Power, Browning, *J. Chem. Soc.* **101**, 2411 (1912). Structure and configuration: Ames *et al.*, *ibid.* **1954**, 1905. Identity with anthesterin: Power, Browning, *ibid.* **105**, 1829 (1914); with  $\alpha$ -lactucerol: Zellner, *Monatsh.* **7**, 681 (1926).



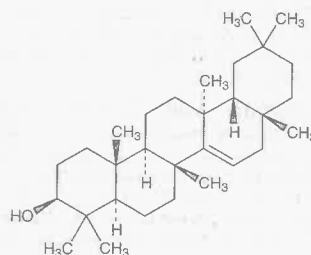
Needles from alcohol, mp 221-222°.  $[\alpha]_D +96.3^\circ$  (CHCl<sub>3</sub>). Very sol in alcohol, ether, petr ether; slightly sol in chloroform, benzene, carbon disulfide, acetone.

**Acetate.** Lactucerin; lactucon.  $C_{32}H_{52}O_2$ . Hexagonal plates, mp 251-252° (from ethyl acetate + alcohol).  $[\alpha]_D +100.5^\circ$ .

**9151. Taraxein.** [9010-30-4] A protein complex isolated from the blood serum of schizophrenics; thought to be an antigenic antibody. Method of isolation: R. G. Heath *et al.*, *Am. J. Psychiatry* **114**, 14 (1957). Studies of relationship to schizophrenia: *idem et al.*, *Arch. Gen. Psychiatry* **16**, 1, 10, 24 (1967); J. R. Bergen *et al.*, *Biol. Psychiatry* **15**, 369 (1980). Review:

R. G. Heath in *Nutrients and Brain Function*, W. B. Essman, Ed. (Karger, Basel, 1987) pp 186-192.

**9152. Taraxerol.** [127-22-0] (3 $\beta$ )-D-Friedoolean-14-en-3-ol; isoolean-14-en-3 $\beta$ -ol; skimmiol; alnulin; tiliadin.  $C_{30}H_{50}O$ ; mol wt 426.72. C 84.44%, H 11.81%, O 3.75%. Found in *Tilia cordata* Mill., *Tiliaceae*: Bräutigam, *Arch. Pharm.* **238**, 555 (1900); in *Alnus glutinosa* (L.) Gaertn., *Betulaceae*: Zellner, Weiss, *Sitzber. Akad. Wiss Wien* **132**, 258 (1923); in *Taraxacum officinale* Weber, *Compositae*: Burrows, Simpson, *J. Chem. Soc.* **1938**, 2042; in *Litsea dealbata* Nees, *Lauraceae*: Dunstan *et al.*, *Aust. J. Chem.* **6**, 321 (1953); from *Befaria racemosa* (Vent.), *Ericaceae*: Euda *et al.*, *J. Org. Chem.* **26**, 271 (1961). Structure: Beaton *et al.*, *J. Chem. Soc.* **1955**, 2131. Partial synthesis from  $\beta$ -amyrin: *idem*, *Chem. & Ind. (London)* **1955**, 35.



Plates from chloroform + methanol, needles from benzene, mp 282-285°. uv max (ethanol): 210, 215, 220, 223 nm ( $\epsilon$  3900, 2400, 700, 250). Sol in benzene, chloroform, ether, ethyl acetate, acetic anhydride, acetic acid, phenol, pyridine, xylene; less sol in alcohol.

**Acetate.**  $C_{32}H_{52}O_2$ . Plates from chloroform + methanol, mp 303-305°.  $[\alpha]_D +10.5^\circ$  (c = 1.8 in chloroform).

**Benzoate.**  $C_{37}H_{54}O_2$ . Needles from benzene or chloroform + alc, mp 292-293°.  $[\alpha]_D^{25} +35.7^\circ$  (c = 0.7 in chloroform).

**9153. Tar Oil.** Volatile oil distilled from wood tar. *Principal constit.* Phenolic substances and hydrocarbons.

Almost colorless liquid when fresh, but soon becomes dark brownish-red. d 0.860-0.900. Insol in water; sol in alcohol. ether.

**9154. Tar Oil, Rectified.** Pine tar oil. The volatile oil from pine tar rectified by steam distillation. Chief active constituents are phenolic substances.

Dark reddish-brown, thin liquid; strong empyreumatic odor and taste.  $d_{25}^{25}$  0.960-0.990. Insol in water; miscible with alcohol.

THERAP CAT: Antiseptic (topical); dermatologic.

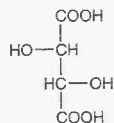
THERAP CAT (VET): Antiseptic, antipruritic. For chronic skin conditions and in hoof dressings. Has been used internally as an expectorant.

**9155. Tarragon.** Estragon. The dried leaves and flowering tops of the perennial herb, *Artemisia dracunculoides* L., *Compositae*. *Habit* Siberia, Caspian Sea region; cultivated in Western Europe. Yields up to 0.8% oil of tarragon. *Constit.* *p*-Allylanisole (estragole; methyl chavicol); ocimene; myrcene; phellandrene(?); *p*-methoxycinnamaldehyde.

USE: The herb for culinary purposes, the oil as flavoring agent in liqueurs, soups, sauces and salad dressings. In perfumery to improve the note of chypre type perfumes.

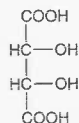
**9156. D-Tartaric Acid.** [147-71-7] (2S,3S)-2,3-Dihydroxybutanedioic acid; unusual tartaric acid; unnatural tartaric acid; *l*-tartaric acid; (-)-tartaric acid; levotartaric acid; D-threo-2,3-dihydroxysuccinic acid.  $C_4H_6O_6$ ; mol wt 150.09. C 32.01%, H 4.03%, O 63.96%. Levorotatory tartaric acid having a dextro configuration. Although termed "unnatural," its occurrence in nature has been demonstrated. Obtained in small amounts from racemic tartaric acid through biochemical cleavage using *Penicillium notatum*, *Aspergillus griseus*, *A. niger* or other microorganisms: Pasteur, *Compt. Rend.* **51**, 298 (1860).

Alternate route using salt formation with *d*-methylamphetamine: Walton, *J. Soc. Chem. Ind.* **64**, 219 (1945). Monograph: K. Freudenberg, *Stereochemie I*, (1933), reprinted by J. W. Edwards (Ann Arbor, 1945). Crystallographic data: A. N. Winchell, *The Optical Properties of Organic Compounds* (Academic Press, New York, 2nd ed., 1954) p 47.



Monoclinic sphenoidal prisms.  $d_4^{20}$  1.7598. mp 168-170°.  $[\alpha]_D^{20}$  -12.0° (c = 20 in H<sub>2</sub>O). pKa<sub>1</sub> 2.93; pKa<sub>2</sub> 4.23. One gram dissolves in 0.75 ml water at room temp, in 0.5 ml boiling water, 1.7 ml methanol, 3 ml ethanol, 0.5 ml propanol, 250 ml ether. Also sol in glycerol. Insol in chloroform. Maximum soly in water at 20°: 139 g/100 ml.

**9157. DL-Tartaric Acid.** [133-37-9] 2,3-Dihydroxybutanedioic acid; racemic tartaric acid; racemic acid; *dl*-tartaric acid; resolvable tartaric acid; uvic acid; paratartaric acid; *dl*-Weinsäure (German); Vogesensäure (German); Traubensäure (German). C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>; mol wt 150.09. C 32.01%, H 4.03%, O 63.96%. Probably never a natural product, although sometimes found in small amounts during wine-making. Prepn from L-tartaric acid by boiling with aq NaOH (*meso*-tartaric acid is obtained as a byproduct): Holleman, *Org. Syn.* **6**, 82 (1926); **coll. vol. I** (2nd ed., 1941) p 497. Synthesis by oxidation of fumaric acid: Milas, Terry, *J. Am. Chem. Soc.* **47**, 1412 (1925); Milas, Sussman, *ibid.* **58**, 1302 (1936); US 2000213 (1935 to Standard Brands). From maleic acid: Church, Blumberg, *Ind. Eng. Chem.* **43**, 1780 (1951).

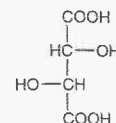


Anhydr acid, triclinic pinacoidal crystals from abs alc, from water above 73°, or by drying the monohydrate at 100°. mp 206°. pKa<sub>1</sub> 2.96; pKa<sub>2</sub> 4.24. Less soluble in water than L-tartaric acid. pH of 0.1M aq soln: 2.0. Soly in alcohol (g/100 g): 2.006 at 0°; 3.153 at 15°; 5.01 at 25°; 6.299 at 40°. Soly in ether about 1%.

**Monohydrate.** Triclinic pinacoidal crystals from water.  $d_4^{20}$  1.697. One hundred parts (w/w) of water dissolve 14.00 parts at 10°; 20.60 at 20°; 29.10 at 30°; 43.32 at 40°; 99.88 at 70°; 184.91 at 100°.

**9158. L-Tartaric Acid.** [87-69-4] (2*R*,3*R*)-2,3-Dihydroxybutanedioic acid; ordinary tartaric acid; natural tartaric acid; *d*-tartaric acid; (+)-tartaric acid; dextrotartaric acid; L-2,3-dihydroxybutanedioic acid; *d*- $\alpha$ , $\beta$ -dihydroxysuccinic acid; Weinsäure (German); Weinsteinssäure (German). C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>; mol wt 150.09. C 32.01%, H 4.03%, O 63.96%. Dextrorotatory tartaric acid having a levo configuration. Widely distributed in nature, classified as a fruit acid. Occurs in many fruits, free and combined with potassium, calcium or magnesium. Observed in antiquity as the acid potassium salt found deposited as a fine crystalline crust during fermentation of grape juice or tamarind juice and termed *faecula* (little yeast) by the Romans. The derivation from *Tartarus* is of medieval, alchemical origin. In modern processes the acid potassium tartrate obtained during wine-making is first converted to calcium tartrate which is then hydrolyzed to tartaric acid and calcium sulfate: Metzner, *Chem. Eng. Progress* **43**, 160 (1947); several modifications, e.g., IT 490221 (1954 to Procedimenti Chimici), C.A. **50**, 11607c (1956). Extraction from tamarind pulp in about 10% yield: IN 52167 (1955), C.A. **50**, 5249g (1956). Synthesis by hydroxyl-

ation of maleic acid: Church, Blumberg, *Ind. Eng. Chem.* **43**, 1780 (1951). Practically all of the L-tartaric acid sold today is a byproduct of the wine industry. Monograph: U. Roux, *La Grande Industrie des Acides Organiques* (Dounod, Paris, 1939). Example of a modern process: Dabul, US 3114770 (1963 to Orandi & Massera).

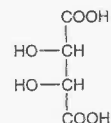


Monoclinic sphenoidal prisms, mp 168-170°. Stable to air and light. Strong acid taste. Refreshing when in dil aq soln.  $d_4^{20}$  1.7598. Odor of burnt sugar when heated to mp.  $[\alpha]_D^{20}$  +12.0° (c = 20 in H<sub>2</sub>O). Strong organic acid. At 25° pKa<sub>1</sub> 2.96, pKa<sub>2</sub> 4.34. pH of 0.1N soln: 2.2. Heat of combustion: -275.1 kcal/mol. Specific heat: 0.288 cal/g°C at 21 to 51°; 0.296 at 0 to 99.6°. Dielectric constant 36.0 for 1200 cm waves. Freely sol in water.  $d_4^{15}$  of aq solns (w/w at 15°): 1% 1.0045; 10% 1.0469; 20% 1.0969; 30% 1.1505; 40% 1.2078; 50% 1.2696. Max soly in water in g/100 ml at various temps: 0° = 115; 10° = 126; 20° = 139; 30° = 156; 40° = 176; 50° = 195; 60° = 217; 70° = 244; 80° = 273; 90° = 307; 100° = 343. One gram dissolves in 0.75 ml water at room temp, in 0.5 ml boiling water, 1.7 ml methanol, 3 ml ethanol, 10.5 ml propanol, 250 ml ether. Also sol in glycerol. Insol in chloroform.

**Caution:** Can cause local irritation. See *Paaty's Industrial Hygiene and Toxicology vol. 2C*, G. D. Clayton, F. E. Clayton, Eds. (Wiley-Interscience, New York, 3rd ed., 1982) p 4937, 4943-4945.

**USE:** In the soft drink industry, confectionery products, bakery products, gelatin desserts, as an acidulant. In photography tanning, ceramics, manuf tartrates. The common commercial esters are the diethyl and dibutyl derivs used for lacquers and in textile printing. Pharmaceutical acid (buffering agent).

**9159. meso-Tartaric Acid.** [147-73-9] Mesotartaric acid; internally compensated tartaric acid; unresolvable tartaric acid; Antiweinsäure (German). C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>; mol wt 150.09. C 32.01%, H 4.03%, O 63.96%. Prepd by boiling L-tartaric acid with alkali; as byproduct of racemization: Winther, *Z. Physik. Chem.* **56**, 507 (1906); Holleman, *Org. Syn. coll. vol. I* (2nd ed., 1941) p 497; Milas, US 2414385 (1947). Microbial prepn: Martin, Foster, *J. Bacteriol.* **70**, 405 (1955); Foster, US 2947665 (1960). Explanation of optical inactivity: Noller, *Science* **102**, 508 (1945); C. R. Noller, *Chemistry of Organic Compounds* (Philadelphia, 2nd ed., 1957) p 339.



**Monohydrate.** Rectangular plates,  $d_4^{20}$  1.666 (also reported as 1.737). mp 140° (also reported as 159-160°). pKa<sub>1</sub> 3.11; pKa<sub>2</sub> 4.80. Maximum soly in water at 20°: 125 g/100 ml.

**9160. Tartrazine.** [1934-21-0] 4,5-Dihydro-5-oxo-1-(4-sulfophenyl)-4-[(4-sulfophenyl)azo]-1*H*-pyrazole-3-carboxylic acid trisodium salt; C.I. Acid Yellow 23; 3-carboxy-5-hydroxy-1-*p*-sulfophenyl-4-*p*-sulfophenylazopyrazole trisodium salt; 5-hydroxy-1-(*p*-sulfophenyl)-4-[(*p*-sulfophenyl)azo]pyrazole-3-carboxylic acid trisodium salt; hydrazine yellow; C.I. 19140; FD & C Yellow No. 5; C.I. Food Yellow 4. C<sub>16</sub>H<sub>9</sub>N<sub>3</sub>Na<sub>3</sub>O<sub>7</sub>S<sub>3</sub>; mol wt 534.37. C 35.96%, H 1.70%, N 10.48%, Na 12.91%, O 26.95%, S 12.00%. Prepn: US 2457823 (1949 to Ilford). Freeman *et al.*, *J. Assoc. Offic. Agr. Chem.* **33**, 937 (1950). See also *Colour Index vol. 4* (3rd ed., 1971) p 4132.