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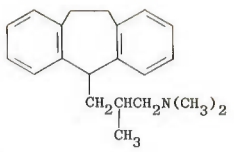
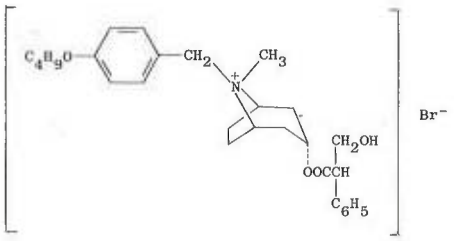


Oil, bp_1 180-185°.

Hydrochloride, $C_{21}H_{28}ClN$, *AY-62014, Evadyne.* Crystals from isopropyl alcohol-ether, mp 188-190° (dec). uv max (methanol): 273, 270, 266 nm (ε 460, 441, 552). Freely sol in water; moderately sol in aliphatic alc, chloroform. Insol in ether, paraffinic hydrocarbons. LD_{50} in mice: 120 mg/kg i.p.; 345 mg/kg orally, Voith, Herr, *Arch. Int. Pharmacodyn Ther.* **182,** 318 (1969).

THERAP CAT: Antidepressant.

1507. Butropium Bromide. *8-[(4-Butoxyphenyl)methyl]-3-(3-hydroxy-1-oxo-2-phenylpropoxy)-8-methyl-8-azoniabicyclo[3.2.1]octane bromide; 8-(p-butoxybenzyl)-3α-hydroxy-1αH,5αH-tropanium bromide (−)-tropate; l-*[1-(*p*-*n*-butoxybenzyl)hyoscyaminium] bromide; BHB; Coliopan. $C_{28}H_{38}BrNO_4$; mol wt 532.53. C 63.15%, H 7.19%, Br 15.00%, N 2.63%, O 12.02%. Prepn: Tanaka, Hashimoto, **Ger.** pat. **1,950,378** (1970) corresp to **U.S.** pat. **3,696,110** (1972); **Japan.** pat. **22,715('72),** *C.A.* **77,** 79549g (1972), (all to Eisai); Tanaka *et al., J. Pharm. Soc. Japan* **92,** 510 (1972). Prepn of the labelled compound: Fujita *et al., J. Label. Compounds* **9,** 149, 555 (1972). Activity: Akutsu, Ichikawa, *Showa Igakkai Zasshi* **32,** 494 (1972), *C.A.* **78,** 119243g (1973). *Review: Japan. Med. Gaz.* **11**(9), 10 (1974).



Crystals from ethanol-acetone, mp 166-168°; also reported as white needles from isopropanol, mp 158-160° (**U.S.** pat. **3,696,110).** $[\alpha]_D^{20}$ −21.7° (c = 0.5 in water). Freely sol in glacial acetic acid; sol in chloroform, DMF. Sparingly sol in ethanol; slightly sol in water, 0.1*N* HCl, 0.1*N* NaOH. Practically insol in acetone, ether, benzene. LD_{50} in male mice (mg./kg): 1500 orally; 660 s.c.; 12.0 i.v., **U.S.** pat. **3,696,110.**

THERAP CAT: Antispasmodic; anticholinergic.

1508. *n*-Butyl Acetate. *Acetic acid butyl ester.* $C_6H_{12}O_2$; mol wt 116.16. C 62.04%, H 10.41%, O 27.55%. $CH_3COO(CH_2)_3CH_3$. Prepd from acetic acid and butyl alcohol: Leyes, Othmer, *Ind. Eng. Chem.* **37,** 968 (1945); Vogel, *J. Chem. Soc.* **1948,** 624; Zettlemoyer *et al.*, **U.S.** pat. **2,644,839** (1953 to FMC); Faith, Keyes & Clark's *Industrial Chemicals,* F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 171-177.

Liquid. d_{20}^{20} 0.8826. bp 125-126°. Solidif −77°. n_D^{20} 1.3951. Flash pt, closed cup: 72° F (22° C). Sol in about 120 parts water at 25°; misc with alcohol, ether; sol in most hydrocarbons. LD_{50} orally in rats: 14.13 g/kg, H. F. Smyth *et al., Arch. Ind. Hyg. Occup. Med.* **10,** 61 (1954).

USE: Manuf lacquer, artificial leather, photographic films, plastics, safety glass. *Caution:* Irritating; may cause conjunctivitis. Narcotic in high concns: E. Browning, *Toxicity and Metabolism of Industrial Solvents* (Elsevier, New York, 1965) pp 529-532, 591-593.

1509. *sec*-Butyl Acetate. *Acetic acid 1-methylpropyl ester; acetic acid sec-butyl ester.* $CH_3COOCH(CH_3)CH_2CH_3$. Empirical formula, mol wt, etc.: *see n*-butyl acetate above. Prepd from *sec*-butanol and acetic anhydride: Altschul, *J. Am. Chem. Soc.* **68,** 2605 (1946). Prepn of *d*-form: Kenyon *et al., J. Chem. Soc.* **1935,** 1072; Bird, *Tetrahedron* **18,** 1 (1962). Prepn of *l*- form: Kenyon *et al., loc. cit.* Manuf: Faith, Keyes & Clark's *Industrial Chemicals,* F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 171-177.

dl-Form, liquid. d_4^{25} 0.865. bp 112-113°. n_D^{25} 1.3866. Flash pt, open cup: 88° F (31° C). Slightly sol in water; sol in alcohol, ether.

d-Form, liquid, bp 116-117°. d_4^{19} 0.873. n_D^{18} 1.3899.

1510. *tert*-Butyl Acetate. *Acetic acid 1,1-dimethylethyl ester; acetic acid tert-butyl ester.* $CH_3COOC(CH_3)_3$. Empirical formula, mol wt, etc.: *see n*-butyl acetate above. Prepn: Baker, Bordwell; Hauser *et al., Org. Syn.* **coll. vol. III,** 141, 142 (1955). Manuf from acetic acid and isobutylene: Young, Pare, **U.S.** pat. **3,031,495** (1962 to Sinclair); Wheeler *et al.*, **U.S.** pat. **3,102,905** (1963 to Celanese); Heisler *et al.*, **U.S.** pat. **3,096,365** (1963 to Texaco); Faith, Keyes & Clark's *Industrial Chemicals,* F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 171-177.

Liquid, bp 97.8°. d_4^{20} 0.8665, d_4^{25} 0.8593. n_D^{20} 1.3870. Practically insol in water; miscible with alcohol, ether.

USE: As gasoline additive (Wheeler *et al., loc. cit.).*

1511. *tert*-Butylacetic Acid. *3,3-Dimethylbutanoic acid; 3,3-dimethylbutyric acid.* $C_6H_{12}O_2$; mol wt 116.16. C 62.04%, H 10.41%, O 27.55%. $(CH_3)_3CCH_2COOH$. Prepn: Homeyer *et al., J. Am. Chem. Soc.* **55,** 4209 (1933); Botterson, Shulman, *J. Org. Chem.* **27,** 1059 (1962); A. Nilsson, R. Carlson, *Acta Chem. Scand.* **B34,** 621 (1980).

Liquid, bp_{26} 96°, bp_{739} 183.0-183.3°, bp 190°. mp 6-7°. fp −11°. n_D^{20} 1.4115 (Botterson, Shulman), also reported as 1.4096 (Homeyer *et al.*). d_4^{20} 0.9124.

1512. *n*-Butyl Acrylate. *2-Propenoic acid butyl ester;* acrylic acid *n*-butyl ester. $C_7H_{12}O_2$; mol wt 128.17. C 65.59%, H 9.44%, O 24.97%. $CH_2{=}CHCOOC_4H_9$. Prepn from *n*-butanol and methyl acrylate: Rehberg, *Org. Syn.* **coll. vol. III,** 146 (1955).

Liquid. d_4^{20} 0.8986; d_4^{15} 0.9110; d_4^{12} 0.9117; d_4^0 0.9202. bp_{760} 145° (also reported 138°); bp_{101} 84-86°; bp_{25} 59°; bp_{10} 39°; bp_8 35°. n_D^{20} 1.4190; n_D^{12} 1.4254. Sp heat (−60°): 0.467 cal/g/°C; heat of vaporization 8.11 kcal/mol; heat of combustion 974.46 kcal/mol. Soly in water at 20°: 0.14 g/100 ml; at 40°: 0.12 g/100 ml. Soly of water in *n*-butyl acrylate at 20°: 0.8 ml/100 g. LD_{50} orally in rats: 3.73 g/kg, H. F. Smyth *et al., Arch. Ind. Hyg. Occup. Med.* **4,** 119 (1951).

Polymer, elastic, tacky substance. Brittle temp −45°.

USE: The monomer in the manuf of polymers and resins for textile and leather finishes, paint formulations, etc.

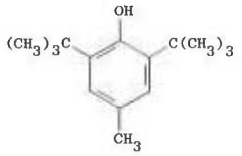
1513. *n*-Butyl Alcohol. *1-Butanol; butyl alcohol;* propyl carbinol. $C_4H_{10}O$; mol wt 74.12. C 64.81%, H 13.60%, O 21.59%. $CH_3CH_2CH_2CH_2OH$. Prepn by reduction of butyraldehyde with sodium borohydride: Chaikin, Brown, *J. Am. Chem. Soc.* **71,** 122 (1949). Manuf from ethylene oxide and triethylaluminum: Rudner, **U.S.** pat. **3,091,627** (1963 to Koppers); by oxidation of tributylborane: Mirviss, **U.S.** pat. **3,067,235** (1962 to Esso). Manuf by carbohydrate fermentation, by hydrogenation of butyraldehyde, from crotonaldehyde: Faith, Keyes & Clark's *Industrial Chemicals,* F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 178-185. Purification and vapor pressure: Biddiscombe *et al., J. Chem. Soc.* **1963,** 1954.

Highly refractive liquid; burns with a strongly luminous flame; leaves a transitory greasy spot on paper. Odor similar to that of fusel oil, but weaker. Its vapors irritate and cause cough. d_4^{20} 0.810. bp 117-118°. mp −90°. Flash pt 36-38°. n_D^{20} 1.3993. A mixture of 63% of the alcohol and 37% water forms a constant boiling mixture, boiling at 92°. Soly at 25°, 9.1 ml/100 ml H_2O: Booth, Everson, *Ind. Eng. Chem.* **40,** 1491 (1948). Miscible with alc, ether and many other organic solvents. LD_{50} orally in rats: 4.36 g/kg, Smyth *et al., Arch. Ind. Hyg. Occup. Med.* **4,** 119 (1951).

USE: As solvent for fats, waxes, resins, shellac, varnish, gums etc.; manuf lacquers, rayon, detergents, other butyl compds; in microscopy for preparing paraffin imbedding materials. *Caution:* May cause irritation of mucous membranes, contact dermatitis, headache, dizziness, drowsiness.

1514. *sec*-Butyl Alcohol. *2-Butanol;* butylene hydrate;

Prepared from *p*-cresol and isobutylene: Stillson, U.S. pat. **2,428,745** (1947 to Gulf); McConnell, Davis, U.S. pat. **3,082,258** (1963 to Eastman Kodak). Inactivator of lipid-containing mammalian and bacterial viruses: Snipes *et al.*, *Science* **188,** 64 (1975).



Crystals, mp 70°. d_4^{20} 1.048. bp 265°. Flash pt (open cup): 260°F (127°C). Insol in water. Freely sol in toluene, sol in methanol, ethanol, isopropanol, methyl ethyl ketone, acetone, Cellosolve, petr ether, benzene, most other hydrocarbon solvents. Soly in liquid petrolatum (white oil): 0.5% w/w. More sol in food oils and fats than butylated hydroxyanisole. Good soly in linseed oil. LD_{50} orally in mice: 1040 mg/kg, *J. Am. Pharm. Assoc.* **38,** 366 (1949).

USE: Antioxidant for food, animal feed, petrol products, synthetic rubbers, plastics, animal and vegetable oils, soaps. Antiskinning agent in paints and inks.

1522. *n*-Butylbenzene. 1-Phenylbutane. $C_{10}H_{14}$; mol wt 134.21. C 89.49%, H 10.51%. $C_6H_5(CH_2)_3CH_3$. Prepn: Radziszewski, *Ber.* **9,** 261 (1876); Balbiano, *Ber.* **10,** 296 (1877); Read, Foster, *J. Am. Chem. Soc.* **48,** 1606 (1926).

Liquid. mp −88.5°. d_4^{20} 0.8604. bp_{760} 183.1°; bp_{400} 159.2°; bp_{200} 136.9°; bp_{100} 116.2°; bp_{60} 102.6°; bp_{40} 92.4°; bp_{20} 76.3°; bp_{10} 62.0°; bp_5 48.8°; $bp_{1.0}$ 22.7°. n_D^{20} 1.49040. Flash pt, open cup: 160° F (71° C). Insol in water; miscible with alcohol, ether, benzene.

1523. *sec*-Butylbenzene. *(1-Methylpropyl)benzene;* 2-phenylbutane. $C_{10}H_{14}$; mol wt 134.21. C 89.49%, H 10.51%. $C_6H_5CH(CH_3)CH_2CH_3$. Prepd from benzene and *n*-butyl chloride in presence of $AlCl_3$: Schramm, *Monatsh.* **9,** 621 (1888); by the action of sodium on γ-chloro-*sec*-butylbenzene: Braun *et al., Ber.* **46,** 1277 (1913); with other products by heating *n*- or *sec*-butyl alcohol with 80% H_2SO_4: Meyer, Bernhauer, *Monatsh.* **53,** 727 (1929).

Liquid. mp −82.7°. d_4^{20} 0.8608. bp_{760} 173.5°; bp_{400} 150.3°; bp_{200} 128.8°; bp_{100} 109.5°; bp_{60} 96.0°; bp_{40} 86.2°; bp_{20} 70.6°; bp_{10} 57.0°; bp_5 44.2°; $bp_{1.0}$ 18.6°. n_D^{20} 1.48980. Flash pt, closed cup: 126° F (52° C). Insol in water; misc with alcohol, ether, benzene.

d-Form, $[\alpha]_D^{25}$ +26.6°: Bonner, Greenlee, *J. Am. Chem. Soc.* **81,** 3336 (1959).

l-Form, $[\alpha]_D^{25}$ −27.3°.

USE: Solvent; in organic syntheses.

1524. *tert*-Butylbenzene. *(1,1-Dimethylethyl)benzene;* 2-methyl-2-phenylpropane; trimethylphenylmethane; pseudobutylbenzene. $C_{10}H_{14}$; mol wt 134.21. C 89.49%, H 10.51%. $C_6H_5C(CH_3)_3$. Prepn: Konowalow, *Bull. Soc. Chim.* [3] **16,** 865 (1896); Shoesmith, Mackie, *J. Chem. Soc.* **1928,** 2336; Meyer, Bernhauer, *Monatsh.* **53,** 727 (1929); Wilt, Abegg, *J. Org. Chem.* **33,** 923 (1968). *See also* Groose, Ipatieff, *J. Am. Chem. Soc.* **57,** 2415 (1935); Ipatieff, Pines, *ibid.* **58,** 1056 (1936).

Liquid. mp −58.1°. d_4^{20} 0.8669. bp_{760} 168.5°; bp_{400} 145.8°; bp_{200} 123.7°; bp_{100} 103.8°; bp_{60} 90.6°; bp_{40} 80.8°; bp_{20} 65.6°; bp_{10} 51.7°; bp_5 39.0°; $bp_{1.0}$ 13.0°. n_D^{20} 1.49235. Flash pt, open cup: 140°F (60°C). Insol in water; misc with alcohol, ether, benzene.

1525. *n*-Butyl Benzoate. *Benzoic acid butyl ester.* $C_{11}H_{14}O_2$; mol wt 178.22. C 74.13%, H 7.92%, O 17.95%. $C_6H_5COO(CH_2)_3CH_3$. Prepn: Newman, Fones, *J. Am. Chem. Soc.* **69,** 1046 (1947); Justoni, **Brit.** pat. **719,891** (1954 to Vismara).

Thick, oily liquid. d 1.00. mp −22°. bp 250°. Practically insoluble in water; sol in alcohol or ether. LD_{50} orally in rats: 5.14 g/kg, Smyth *et al., Arch. Ind. Hyg. Occup. Med.* **10,** 61 (1954).

1526. *n*-Butyl Bromide. *1-Bromobutane.* C_4H_9Br; mol wt 137.03. C 35.06%, H 6.62%, Br 58.32%. $CH_3(CH_2)_3Br$. Prepd from *n*-butyl alc and a hydrobromic-sulfuric acid mixture: Kamm, Marvel, *Org. Syn.* **vol. 1,** 5 (1921); Skau, McCullough, *J. Am. Chem. Soc.* **57,** 2440 (1935).

Colorless liquid. d_4^{25} 1.2686. bp_{760} 101.3° (mp −112°). n_D^{20} 1.4398. Insol in water; sol in alcohol, ether.

1527. *sec*-Butyl Bromide. *2-Bromobutane;* methylethylbromomethane. C_4H_9Br; mol wt 137.03. C 35.06%, H 6.62%, Br 58.32%. $CH_3CH_2CHBrCH_3$. Prepn: Levene, Marker, *J. Biol. Chem.* **91,** 405 (1931); Kenyon *et al., J. Chem. Soc.* **1935,** 1080; Skau, McCullough, *J. Am. Chem. Soc.* **57,** 2440 (1935); Colson *et al., J. Chem. Soc.* **1965,** 2364. Prepn of optically pure isomers: Goodwin, Hudson, *J. Chem. Soc. (B)* **1968,** 1333.

dl-Form, colorless liquid, pleasant odor. d_4^{25} 1.2530. bp 91.2° (mp −112°). n_D^{25} 1.4344. Insol in water. Freely sol in alcohol, ether.

d-Form, n_D^{20} 1.4359-1.4362. α_D^{20} +42.64°.

l-Form, n_D^{20} 1.4368. α_D^{20} −43.7°.

Caution: Narcotic in high concns.

1528. *tert*-Butyl Bromide. *2-Bromo-2-methylpropane;* 2-bromoisobutane; trimethylbromomethane. C_4H_9Br; mol wt 137.03. C 35.06%, H 6.62%, Br 58.32%. $(CH_3)_3CBr$. Prepn: Brunel, *J. Am. Chem. Soc.* **39,** 1978 (1917); Bryce-Smith, Howlett, *J. Chem. Soc.* **1951,** 1141; Coe *et al., ibid.* **1954,** 2281.

Colorless liquid. d_4^{25} 1.2125. bp 73.3°. fp −16.3°. At 210° changes to isobutyl bromide. n_D^{25} 1.4249. Insol in water; miscible with organic solvents.

1529. *n*-Butyl *n*-Butyrate. *Butanoic acid butyl ester; butyric acid butyl ester.* $C_8H_{16}O_2$; mol wt 144.21. C 66.63%, H 11.18%, O 22.19%. $CH_3(CH_2)_2COO(CH_2)_3CH_3$. Prepn from butyl alcohol: Robertson, *Org. Syn.* **coll. vol. I,** 138 (1941); Horton, U.S. pat. **2,522,676** (1950 to Socony-Vacuum Oil).

Liquid, bp 165°. d_4^{20} 0.8692. n_D^{20} 1.4064. Practically insol in water; miscible with alcohol, ether.

1530. Butyl Carbitol®. *2-(2-Butoxyethoxy)ethanol;* diethylene glycol monobutyl ether. $C_8H_{18}O_3$; mol wt 162.22. C 59.23%, H 11.18%, O 29.59%. $HOCH_2CH_2OCH_2CH_2OC_4H_9$. Prepn: Riemschneider, Gross, *Monatsh.* **90,** 783 (1959). Purification: Miller, Yonan, *J. Am. Chem. Soc.* **79,** 5931 (1957); Ridley, Ridley, **Brit.** pat. **795,866** (1958 to Esso).

Practically odorless liquid, bp 230.4°. mp −68.1°. d_{20}^{20} 0.9536. n_D^{27} 1.4258. Miscible in water, oils. Miscibility in other organic solvents: Jackson, Drury, *Ind. Eng. Chem.* **51,** 1491 (1959). Flash pt 110°. LD_{50} orally in rats, guinea pigs: 6.56, 2.00 g/kg, Smyth *et al., J. Ind. Hyg. Toxicol.* **23,** 259 (1941).

1531. *n*-Butyl Carbonate. *Carbonic acid dibutyl ester;* dibutyl carbonate. $C_9H_{18}O_3$; mol wt 174.23. C 62.04%, H 10.41%, O 27.55%. $(C_4H_9O)_2CO$. Prepn from ethyl carbonate, butyl alcohol and ethylmagnesium bromide: Frank *et al., J. Am. Chem. Soc.* **66,** 1509 (1944); from butyl alcohol and CO in the presence of Pd and $CuCl_2$: Mador, Blackham, U.S. pat. **3,114,762** (1963 to National Distillers).

Liquid, bp 206.6°. d_4^{20} 0.9251, d_4^{25} 0.9388. n_D^{20} 1.4117. Practically insol in water. Miscible with ethanol, benzene, chloroform, acetone, ether and other organic solvents, *see:* Jackson, Drury, *Ind. Eng. Chem.* **51,** 1491 (1959).

1532. Butyl Cellosolve®. *2-Butoxyethanol;* ethylene glycol monobutyl ether. $C_6H_{14}O_2$; mol wt 118.17. C 60.98%, H 11.94%, O 27.08%. $HOCH_2CH_2OC_4H_9$. Prepn from butyl alcohol and ethylene carbonate or 2-chloroethanol, or from ethylene glycol and butyl bromide: Carlson, U.S. pat. **2,448,767** (1948 to Mellon Inst. Ind. Res.); Klamann, Bertsch, *Ber.* **88,** 201 (1955); Riemschneider, Gross, *Monatsh.* **90,** 783 (1959). Toxicity: Carpenter *et al., Arch. Ind. Health* **14,** 114 (1956).

Liquid, bp 171-172°. d_4^{20} 0.9012, d_{20}^{20} 0.9019. n_D^{20} 1.4196. Flash pt, closed cup: 141°F (60°C). Soluble in 20 parts water; sol in most organic solvents, in mineral oil. LD_{50} orally in rats: 1.48 g/kg, H. F. Smyth *et al., J. Ind. Hyg. Toxicol.* **23,** 259 (1941).

USE: Solvent for nitrocellulose, resins, grease, oil, albumin; dry cleaning. *Caution:* Toxic symptoms similar to those for Methyl Cellosolve.