

THE MERCK INDEX
ELEVENTH EDITION

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THE MERCK INDEX

AN ENCYCLOPEDIA OF
CHEMICALS, DRUGS, AND BIOLOGICALS

ELEVENTH EDITION

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Slightly sol in cold water; sol in hot water (yellowish-red soln). Violet-red in conc H_2SO_4 , turning blue on addn of boric acid. Violet in aq NaOH.

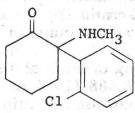
USE: As brilliant scarlet dye.

5173. Kerosene. Kerosine. A mixture of petroleum hydrocarbons, chiefly of the methane series having from 10 to 16 carbon atoms per molecule. It constitutes the fifth fraction in the distillation of petroleum (after the petr ethers and before the oils). A typical analysis of the kerosene fraction from Midcontinent crude includes *n*-dodecane, three alkyl derivatives of benzene, naphthalene, 1- and 2-methyl-5,6,7,8-tetrahydronaphthalene.

Pale yellow or water-white, mobile, oily liquid. Characteristic, not altogether disagreeable odor. d about 0.80. bp 175-325°. Flash pt 150-185°F. (65-85°C). Insol in water. Misc with other petroleum solvents. A water-white, deodorized form of kerosene is marketed under the trade name *Deobase*. Kerosene is deodorized and decolorized by washing with (fuming) sulfuric acid, followed by sodium plumbite soln and sulfur (Doctor sweetening). LD₅₀ orally in rabbits: 28 ml/kg, W. B. Deichmann *et al.*, *Ann. Int. Med.* **21**, 803 (1944).

USE: In kerosene lamps, flares, and stoves; as degreaser and cleaner; *Deobase* formerly used as a solvent in cosmetics and in fly spray. *Human Toxicity:* Defatting action on skin can lead to irritation, infection. Inhalation of high concns causes headache, drowsiness, coma. Swallowing causes G.I. irritation with vomiting, diarrhea. Aspiration of vomitus causes serious pneumonitis. Toxicological studies and recommended treatment of kerosene poisoning: H. W. Gerarde, *Toxicol. Appl. Pharmacol.* **1**, 462 (1959). *Caution:* Induction of vomiting following ingestion is contraindicated.

5174. Ketamine. (\pm)-2-(2-Chlorophenyl)-2-(methylamino)cyclohexanone; 2-(methylamino)-2-(2-chlorophenyl)-cyclohexanone. C₁₃H₁₆ClNO; mol wt 237.74. C 65.68%, H 6.78%, Cl 14.92%, N 5.89%, O 6.73%. Prepn: Stevens, Belg. pat. 634,208 (1963) corres to U.S. pat. 3,254,124 (1966 to Parke, Davis). Prepn and characterization of T-labelled compd: Blackburn, Ober, *J. Label. Compounds* **3**, 38 (1967). Isoln of optical isomers: Hudyma *et al.*, Ger. pat. 2,062,620 (1971 to Bristol-Myers), C.A. **75**, 118119x (1971). Pharmacology: Domino *et al.*, *Clin. Pharmacol. Ther.* **6**, 279 (1966); Chen *et al.*, *J. Pharmacol. Exp. Ther.* **152**, 332 (1966). Toxicity: E. J. Goldenthal, *Toxicol. Appl. Pharmacol.* **18**, 185 (1971). Comprehensive description: W. C. Sass, S. A. Fusari in *Analytical Profiles of Drug Substances* vol. **6**, K. Florey, Ed. (Academic Press, New York, 1977) pp 297-322.



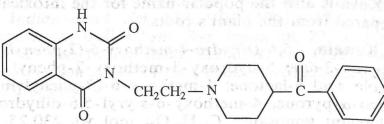
Crystals from pentane-ether, mp 92-93°. uv max (0.01N NaOH in 95% methanol): 301, 276, 268, 261 nm (A_{1cm} 5.0, 7.0, 9.8, 10.5). pKa 7.5.

Hydrochloride, C₁₃H₁₇Cl₂NO, Cl-581, *Ketaject*, *Ketalar*, *Ketanest*, *Ketaset*, *Ketavet*, *Vetalar*. White crystals, mp 262-263°. Soly in water: 20 g/100 ml. LD₅₀ in adult mice, rats (mg/kg): 224 ± 4, 229 ± 5 i.p. (Goldenthal).

THERAP CAT: Anesthetic (intravenous).

THERAP CAT (VET): Anesthetic.

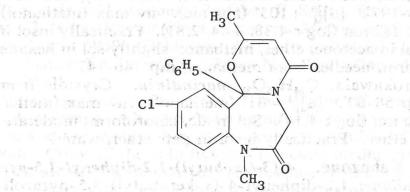
5175. Ketanserin. 3-[2-[4-(4-Fluorobenzoyl)-1-piperidinyl]ethyl]-2,4[1H,3H]-quinazolinodione; R 41468; Ket; Serefrex; Serepress; Surexal. C₂₂H₂₂FN₃O₃; mol wt 395.43. C 66.82%, H 5.61%, F 4.80%, N 10.63%, O 12.14%. Specific serotonin S₂-receptor antagonist with hypotensive properties. Prepn: J. Vandenbeck *et al.*, *Eur. Pat. Appl.* **13**, 612; *ibid.*, U.S. pat. 4,335,127 (1980, 1982 both to Janssen). X-ray structure: O. M. Peeters *et al.*, *Cryst. Struct. Commun.* **11**, 375 (1982). Receptor binding profile, physical properties: J. E. Leyens *et al.*, *Life Sci.* **28**, 1015 (1981). Antihypertensive properties: J. M. Van Neuten *et al.*, *J. Pharmacol. Exp. Ther.* **218**, 217 (1981). Use in treatment of cardiac failure: J.-C. Demoulin *et al.*, *Lancet* **1**, 1186 (1981). HPLC determin in plasma: A. T. Kacprowicz *et al.*, *J. Chromatogr.* **272**, 417 (1983); C. L. Davies, *ibid.* **275**, 232 (1983). Efficacy in treatment of intermittent claudication: J. De Cree *et al.*, *Lancet* **2**, 775 (1984). Long term treatment of hypertensive patients: A. Amery *et al.*, *J. Cardiovasc. Pharmacol.* **6**, 182 (1984). In treatment of Raynaud's phenomenon: E. Strandén *et al.*, *Brit. Med. J.* **285**, 1069 (1982); J. R. Seibold, A. H. M. Jageneau, *Arthritis Rheum.* **27**, 139 (1984). Review of antihypertensive properties: P. M. Vanhoutte *et al.*, *Fed. Proc.* **42**, 182-185 (1983); of pharmacology: J. M. Van Neuten, P. M. Vanhoutte, *Biol. Cardiol.* **38**, 222-233 (1984). Series of articles on cardiovascular effects: *J. Cardiovasc. Pharmacol.* **7**, Suppl. 7, S1-S182 (1985); on pharmacokinetics and metabolism in animals and man: *Arzneimittelforschung* **38**, 775-800 (1988).



Crystals from 4-methyl-2-pentanone, mp 227-235°. Soly (g/100 ml): 0.001 in water; 0.038 in ethanol; 2.34 in DMF. pKa 7.5.

THERAP CAT: Antihypertensive.

5176. Ketazolam. 11-Chloro-8,12b-dihydro-2,8-dimethyl-12b-phenyl-4H-[1,3]oxazolo[3,2-d][1,4]benzodiazepine-4,7(6H)-dione; U-28,774; Anseren; Ansieten; Anxon; Contaxem; Loftram; Unakalm. C₂₀H₁₇ClN₃O₃; mol wt 368.82. C 65.13%, H 4.65%, Cl 9.61%, N 7.59%, O 13.01%. Prepn: J. Szmuszkovicz, Ger. pat. 1,947,226 corres to U.S. pat. 3,573,282 (1970, 1971 both to Upjohn); U.S. pat. 3,575,965 (1971 to Upjohn). Synthesis and structure: J. Szmuszkovicz *et al.*, *Tetrahedron Letters* **1971**, 3665. Analysis by HPLC: D. J. Weber, *J. Pharm. Sci.* **61**, 1797 (1972). Pharmacology: V. H. Sethy, *Arch. Exp. Pathol. Pharmacol.* **301**, 157 (1978). Clinical studies: L. F. Fabre, *J. Inst. Med. Res.* **4**, 50 (1976); L. A. Gottschalk, J. B. Cohn, *Psychopharmacol. Bull.* **14**, 39 (1978).



Colorless prisms from chloroform/ether, mp 182-183.5° (sinters at 170°). uv max (ethanol): 202, 241 nm (ε 40600; 18400).

Note: This is a controlled substance (depressant) listed in the U.S. Code of Federal Regulations, Title 21 Part 1308.14 (1987).

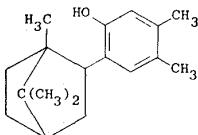
THERAP CAT: Anxiolytic.

5177. Ketene. *Ethenone*; carbomethene. C₂H₂O; mol wt 42.04. C 57.14%, H 4.80%, O 38.06%. CH₂=C=O. Prepd by the thermal decompr of acetone, diketene or acetic anhydride: Hurd, *Org. Syn. coll. vol. I*, 330 (2nd ed., 1941); S. Andreades, H. D. Carlson, *ibid. coll. vol. V*, 679 (1973). Structure of ketene dimer as 3-buteno-β-lactone: Blomquist, Baldwin, *J. Am. Chem. Soc.* **70**, 29 (1948); Hurd, Blanchard, *ibid.* **72**, 1461 (1950); Katz, Lipscomb, *J. Org. Chem.* **17**, 515 (1953). Toxicology: J. F. Treon *et al.*, *J. Ind. Hyg. Toxicol.* **31**, 209 (1949). Review on the prepn of stable ketenes: R. S. Ward in *The Chemistry of Ketenes, Allenes and Related Compounds. Part 1*, S. Patai, Ed. (Wiley, New York, 1980) pp 223-277; on synthetic uses of ketenes: W. T. Brady, *ibid.* pp 279-308.

Gas. Penetrating odor. mp -150°. bp -56°. Electron diffraction pictures: Beach, Stevenson, *J. Chem. Physics* **6**, 75 (1938). Fairly sol in acetone.

Human Toxicity: Poisonous gas of the same order of tox-

Xipamide

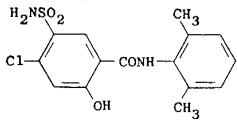


Crystals from petr ether, mp 94-96°; bp₃ 165-168°. Also reported as very viscous, pale yellow liquid; bp₉ 185-189°. d₄²⁰ 1.0240; n_D²⁰ 1.5382 (Starkov, Glushkova).

USE: Rubber antioxidant.

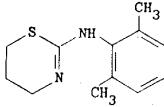
THERAP CAT: Antibacterial.

9986. Xipamide. *4-Chloro-5-sulfamoyl-2',6'-salicyloylidide*; 4-chloro-2',6'-dimethyl-5-sulfamoylsalicyloyl; Bei 1293; Aquaphor; Diurexan; Lumitens. C₁₅H₁₅ClN₂O₄S; mol wt 354.81. C 50.78%, H 4.26%, Cl 9.99%, N 7.89%, O 18.04%, S 9.04%. Salicylic acid derivative. Prepn: Neth. pat. Appl. 6,607,680 corresp to Liebenow, U.S. pat. 3,567,777 (1966 and 1970 to P. Beiersdorf). Clinical studies: O. Hammer, U. Dembowksi, *Med. Klin.* **64**, 1862 (1969); R. Fischer, A. Lenhartz, *Med. Welt* **1970**, 270. Review of pharmacology and therapeutic efficacy: B. N. C. Prichard, R. N. Brogden, *Drugs* **30**, 313-332 (1985).



Crystals from methanol-water, mp 256°. THERAP CAT: Diuretic. Antihypertensive.

9987. Xylazine. *N-(2,6-Dimethylphenyl)-5,6-dihydro-4H-1,3-thiazin-2-amine*; *5,6-dihydro-2-(2,6-xylidino)-4H-1,3-thiazine*; *2-(2,6-dimethylphenylamino)-4H-5,6-dihydro-1,3-thiazine*; BAY 1470; BAY VA 1470; Wh7286; Rompun (also the hydrochloride). C₁₂H₁₆N₂S; mol wt 220.33. C 65.42%, H 7.32%, N 12.71% S 14.55%. Prepn: Behner et al., Ger. pat. 1,173,475 (1964), C.A. **61**, 13323c (1964); eidem, Belg. pat. 634,552 (1964) corresp to U.S. pat. 3,235,550 (1966) (all to Bayer). Pharmacology: G. Sagner et al., *Deut. Tierarztl. Wochenschr.* **75**, 565 (1968); Kroneberg, Schlossman, *Arch. Pharmakol. Exp. Pathol.* **268**, 348 (1971). Metabolic studies: Duhm et al., *Berlin. Münch. Tierarztl. Wochenschr.* **82**, 104 (1969). Veterinary clinical studies: Clarke, Hall, *Vet. Rec.* **85**, 512 (1969); Burns, McMullan, *Vet. Med.* **67**, 77 (1972).



Colorless, almost tasteless crystals from benzene + ligroin, mp 140-142°. Also reported as mp 136-139°. Soluble in dilute acids, benzene, acetone, chloroform; sparingly sol in petr ether. Practically insol in water, alkalies. LD₅₀ in mice (mg/kg): 43 i.v.; 121 s.c.; 240 orally (Sagner).

Hydrochloride, C₁₂H₁₇ClN₂S, crystals from ethanol + ethyl ether, mp 236-239°.

THERAP CAT (VET): Sedative, analgesic, muscle relaxant.

9988. Xylene. *Dimethylbenzene*; *xylol*. C₈H₁₀; mol wt 106.16. C 90.50%, H 9.50%. C₈H₁₀(CH₃)₂. First isolated from a crude wood distillate: Cahours, *Compt. Rend.* **30**, 319 (1850). Obtained from coal tar: Fittig, *Ann.* **153**, 265 (1870). The xylene of commerce is a mixture of the three isomers *o*-, *m*- and *p*-xylene, the *m*-isomer predominating. Manuf from pseudocumene: Seubold, U.S. pat. 2,960,545 (1960 to Union Oil); by catalytic isomerization of a hydrocarbon fraction: Berger, U.S. pat. 3,078,318 (1963 to Universal Oil Prod.). Separation of isomers by clathration: Schaeffer, U.S. pat. 3,029,300 (1962 to Union Oil). Toxicol-

ogy: E. Browning, *Toxicity and Metabolism of Industrial Solvents* (Elsevier, New York, 1965) pp 77-89. Use as clearing agent: K. Kubota, *J. Polym. Sci.* **5**, 1179 (1967); J. B. Matthews, *J. Clin. Pathol.* **34**, 103 (1981). Review of mfg processes: Faith, Keyes & Clark's *Industrial Chemicals*, F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 874-881. Toxicity: H. F. Smyth et al., *Am. Ind. Hyg. Assoc. J.* **23**, 95 (1962).

Mobile, flammable liquid; d about 0.86; bp 137-140°. Flash pt 29°. Practically insol in water. Miscible with abs alcohol, ether, and many other organic liquids.

m-Xylene, colorless liquid; d₄²⁵ 0.8684; mp -47.4°; bp 139.3°; n_D²⁰ 1.4973. Flash pt, closed cup: 77°F (25°C). Insol in water. Miscible with alcohol, ether, and many other organic solvents. LD₅₀ orally in rats: 7.71 ml/kg (Smyth).

o-Xylene, colorless liquid; d₄²⁰ 0.8801; mp -25°; bp 144°; n_D²⁰ 1.5058. Flash pt, closed cup: 63°F (17°C). Insol in water. Miscible with alc, ether.

p-Xylene, colorless plates or prisms at low temp; d₄²⁰ 0.86104; mp 13-14°; bp 137-138°; n_D²⁰ 1.49575; Thorne et al., *Ind. Eng. Chem. Anal. Ed.* **17**, 481 (1945). Flash pt, closed cup: 77°F (25°C). Insol in water. Sol in alcohol, ether, and many other organic solvents.

Caution: May be narcotic in high concns. Chronic toxicity not well defined, but is less toxic than benzene.

USE: As solvent; raw material for production of benzoic acid, phthalic anhydride, isophthalic and terephthalic acids as well as their dimethyl esters used in the manufacture of polyester fibers; manuf dyes and other organics; sterilizing catgut; with Canada balsam as oil-immersion in microscopy; clearing agent in microscope technique.

9989. Xylenol. *Dimethylphenol*. C₈H₁₀O; mol wt 122.16. C 78.65%, H 8.25%, O 13.10%. (CH₃)₂C₆H₃OH. Constituent of "cresylic acid." There are 6 isomers of xylenol. They are only slightly sol in water but freely sol in alcohol, chloroform, ether, benzene, etc.; also sol in NaOH soln. Prepn and physical properties: R. J. L. Andon et al., *J. Chem. Soc.* **1960**, 5246.

2,3-Dimethylphenol, *vic-o-xylenol*. Needles from water or dil alc, mp 75°, bp 218°. Thööl, *Ber.* **18**, 2561 (1885); also reported as mp 72.57° ± 0.02°. bp₇₆₀ 216.87° ± 0.001° (Andon).

2,4-Dimethylphenol, *as-m-xylenol*. Crystals, bp₇₆₀ 211.5°; mp 25.4-26°. Jacobsen, *Ber.* **11**, 17 (1887); **18**, 3463 (1885); also reported as mp 24.54° ± 0.01°. bp₇₆₀ 210.931° ± 0.001° (Andon).

2,5-Dimethylphenol, *p-xylenol*. Crystals from alcohol + ether, mp 74.5°, bp₇₆₀ 211.5°. Jacobsen, *loc. cit.* bp 213.5°. Würtz, *Ann.* **147**, 372 (1868); also reported as mp 74.85° ± 0.02°. bp₇₆₀ 211.132° ± 0.002° (Andon).

2,6-Dimethylphenol, *vic-m-xylenol*. Needles, mp 49°, bp 203°. Gattermann, *Ann.* **357**, 313 (1907); also reported as mp 45.62° ± 0.01°. bp₇₆₀ 201.030° ± 0.001° (Andon).

3,4-Dimethylphenol, *as-o-xylenol*. Needles from water, mp 62.5°, bp 225°. Jacobsen, *Ber.* **17**, 159 (1884); also reported as mp 65.11° ± 0.01°. bp₇₆₀ 226.947° ± 0.001° (Andon).

3,5-Dimethylphenol, *sym-m-xylenol*. Needles from water, mp 64°, bp 219.5°. Thööl, *Ber.* **18**, 359 (1885); also reported as mp 63.27° ± 0.02°. bp₇₆₀ 221.962° ± 0.003° (Andon).

USE: For the prep of coal tar disinfectants; manuf of artificial resins.

9990. Xylenol Blue. *4,4'-(3H-2,1-Benzoxathiol-3-ylidene)bis[2,5-dimethylphenol] S,S-dioxide*; *p-xylenolsulfone-phthalain*; *1,4-dimethyl-5-hydroxybenzenesulfonephthalain*; *α,4,4'-trihydroxy-2,5,2',5'-tetramethyltriphenylmethane*.

