



>>Entry Name: 2-Ethyl-1,3-hexanediol, 9CI

Synonym(s): Ethohexadiol. Octylene glycol

CAS Registry Number: 94-96-2

H3CCH2CH2CH(OH)CH(CH2OH)CH2CH3

Molecular Formula: C₈H₁₈O₂

Molecular Weight: 146.229

Accurate Mass: 146.13068

Percentage Composition: C 65.71%; H 12.41%; O 21.88%

Use/Importance: Insect repellent. Now superseded

Physical Description: Liq.

Melting Point: Mp -40°

Boiling Point: Bp 244°

Solubility: Sl. sol. H₂O, misc. CHCl₃, EtOH, Et₂O

Density: d₂₀²⁰ 0.942

Refractive Index: n_D²⁰ 1.4511

Other Data: Mixt. of diastereoisomers

Hazard & Toxicity: Fl. p. >110°, autoignition temp. 360°. Mod. toxic orally

Aldrich: E2912-5

Fluka: 4020

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 203C, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 135A, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 196D, (ir)

Kulpinski, M.J. *et al.*, *J.O.C.*, 1943, **8**, 256, (synth)

U.S. Pat., 1943, 2 407 205; *CA*, **41**, 1382a, (use)

King, W.V., *J. Econ. Entomol.*, 1951, **44**, 339, (rev)

Travis, B.V. *et al.*, *J. Econ. Entomol.*, 1951, **44**, 428, (rev)

Blanc, P.Y. *et al.*, *Helv. Chim. Acta*, 1964, **47**, 567, (synth)

Pochini, A. *et al.*, *Synthesis*, 1975, 164, (synth)

Pesticide Manual, 9th edn., 1991, No. 5830

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, EKV000