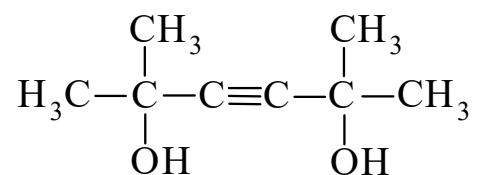




>>Entry Name: 2,5-Dimethyl-3-hexyne-2,5-diol, 9CI



CAS Registry Number: 142-30-3

Molecular Formula: C₈H₁₄O₂

Molecular Weight: 142.197

Accurate Mass: 142.09938

Percentage Composition: C 67.57%; H 9.92%; O 22.50%

Physical Description: Cryst. (C₆H₆ or Et₂O)

Melting Point: Mp 97°

Boiling Point: Bp 205°

Solubility: Sl. sol. H₂O; sol. Me₂CO, EtOH, EtOAc

Aldrich: 22262-3

>>Derivative: Di-Ac

CAS Registry Number: 34106-07-5

Molecular Formula: C₁₂H₁₈O₄

Molecular Weight: 226.272

Accurate Mass: 226.12051

Percentage Composition: C 63.70%; H 8.02%; O 28.28%

Physical Description: Liq.

Boiling Point: Bp₁₄ 112°

>>Derivative: Dibenzoyl

Molecular Formula: C₂₂H₂₂O₄

Molecular Weight: 350.413

Accurate Mass: 350.15181

Percentage Composition: C 75.41%; H 6.33%; O 18.26%

Physical Description: Cryst.

Melting Point: Mp 113-115°

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **3**, 515B, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 939C, (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1589B, (*ir*)
Besserre, D., *Bull. Soc. Chim. Fr.*, 1959, 1596, (*synth*)
Shimao, I. *et al.*, *Nippon Kagaku Zasshi*, 1965, **86**, 1085; *CA*, **65**, 13525f, (*synth*)
Allen, A.D. *et al.*, *Can. J. Chem.*, 1966, **44**, 2703, (*ir*)
Kaplan, P.D. *et al.*, *Inorg. Chem.*, 1967, **6**, 1096, (*pmr*)
Rodina, L.L. *et al.*, *Zh. Org. Khim.*, 1970, **6**, 2336; *CA*, **74**, 42236g, (*synth*)