



>>Entry Name: 2,2,4-Trimethyl-1,3-pentanediol, 9CI

CAS Registry Number: 144-19-4

Related CAS Registry Numbers(s): 25265-77-4

$(\text{H}_3\text{C})_2\text{CHCH}(\text{OH})\text{C}(\text{CH}_3)_2\text{CH}_2\text{OH}$

Molecular Formula: $\text{C}_8\text{H}_{18}\text{O}_2$

Molecular Weight: 146.229

Accurate Mass: 146.13068

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

Aldrich: 32722-0

Fluka: 92620

Rare Chemicals Library: S56420-6

>>Variant: ($\pm$)-form

CAS Registry Number: 127894-68-2

Molecular Formula: $\text{C}_8\text{H}_{18}\text{O}_2$

Molecular Weight: 146.229

Accurate Mass: 146.13068

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

Use/Importance: Used as a 1% soln. in CHCl_3 for extraction of B. Used in the synth. of coatings, resins, films, synthetic lubricants, elastomers, and urethane foams

Physical Description: Cryst.

Melting Point: Mp 52-56°

Boiling Point: Bp 232°

Solubility: Sl. sol. H_2O

>>Derivative: Bis(2-methylpropanoyl)

Synonym(s): 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate

CAS Registry Number: 6846-50-0

Molecular Formula: $\text{C}_{16}\text{H}_{30}\text{O}_4$

Molecular Weight: 286.411

Accurate Mass: 286.21441

Percentage Composition: C 67.10%; H 10.56%; O 22.34%

Use/Importance: Plasticiser for PVC

Physical Description: Liq.

Melting Point: Mp -70°

Boiling Point: Bp 280°

Aldrich: 36865-2

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 202A, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 194C, (*ir*)

Francke, A., *Monatsh. Chem.*, 1896, **71**, 85, (*synth*)

Saunders, R.H. *et al.*, *J.A.C.S.*, 1943, **65**, 1714, (*synth*)

Aznarez, J. *et al.*, *Talanta*, 1985, **32**, 1156, (*detn, B*)

Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **12**, 730, (*rev*)

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