



>>Entry Name: 1,7-Heptanediol, 9CI

CAS Registry Number: 629-30-1

HOH₂C(CH₂)₅CH₂OH

Molecular Formula: C₇H₁₆O₂

Molecular Weight: 132.202

Accurate Mass: 132.11503

Percentage Composition: C 63.60%; H 12.20%; O 24.20%

Physical Description: Hygroscopic solid

Melting Point: Mp 22.5°

Boiling Point: Bp 262° (Bp₃ 112-115°)

Solubility: Sol. H₂O, spar. sol. Et₂O

Aldrich: H220-1

Fluka: 51770

Sigma: H0753

>>Derivative: Di-Ac

CAS Registry Number: 52819-34-8

Molecular Formula: C₁₁H₂₀O₄

Molecular Weight: 216.277

Accurate Mass: 216.13616

Percentage Composition: C 61.09%; H 9.32%; O 29.59%

Boiling Point: Bp 274°

>>Derivative: Bisphenylurethane

Melting Point: Mp 137°

>>Derivative: Disulfamoyl

Synonym(s): Hepsulfam. NSC 329680

CAS Registry Number: 96892-57-8

Molecular Formula: C₇H₁₈N₂O₆S₂

Molecular Weight: 290.361

Accurate Mass: 290.060628

Percentage Composition: C 28.96%; H 6.25%; N 9.65%; O 33.06%; S 22.09%

Biological Use/Importance: Alkylating agent, active against mouse and human mammary carcinoma

Physical Description: Granules (EtOAc/hexane)

Melting Point: Mp 87-88°

Other Data: Hydrophilic analogue of Busulfan [CXB41-Q](#)

>>Derivative: Di-Me ether

Synonym(s): 1,7-Dimethoxyheptane

CAS Registry Number: 137333-33-6

Molecular Formula: C₉H₂₀O₂

Molecular Weight: 160.256

Accurate Mass: 160.14633

Percentage Composition: C 67.45%; H 12.58%; O 19.97%

Boiling Point: Bp 201°. Bp₃₈ 108°

References:

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Marshall, M.V. *et al.*, *Stem Cells (Miamisburg, Ohio)*, 1993, **11**, 62-69, (*hepsulfam, phase I clinical trials*)

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Thalladi, V.R. *et al.*, *Angew. Chem., Int. Ed.*, 2000, **39**, 918-922, (*cryst struct*)