



>>Entry Name: 4-Oxoheptanoic acid, 9CI

Synonym(s): Homolevulinic acid

CAS Registry Number: 1117-74-4

$\text{H}_3\text{CCH}_2\text{COCH}_2\text{CH}_2\text{COOH}$

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_3$

Molecular Weight: 130.143

Accurate Mass: 130.062995

Percentage Composition: C 55.37%; H 7.74%; O 36.88%

Physical Description: Leaflets (Et_2O /petrol)

Melting Point: Mp 40°

Boiling Point: Bp₁₆ 143-144°. Bp_{0.4} 89°

Other Data: Hygroscopic

Rare Chemicals Library: S57409-0

>>Derivative: Phenylhydrazone

Melting Point: Mp 152°

>>Derivative: Semicarbazone

Physical Description: Prisms (EtOH)

Melting Point: Mp 186°

>>Derivative: Et ester

CAS Registry Number: 3249-33-0

Molecular Formula: $\text{C}_8\text{H}_{14}\text{O}_3$

Molecular Weight: 158.197

Accurate Mass: 158.094295

Percentage Composition: C 60.74%; H 8.92%; O 30.34%

Boiling Point: Bp₁₄ 91°

>>Derivative: Et ester, semicarbazone

Physical Description: Needles (EtOAc/petrol)

Melting Point: Mp 142° (106°)

>>Derivative: Nitrile

Synonym(s): 1-Cyano-3-pentanone

CAS Registry Number: 14274-30-7

Molecular Formula: $\text{C}_6\text{H}_9\text{NO}$

Molecular Weight: 111.143

Accurate Mass: 111.068414

Percentage Composition: C 64.84%; H 8.16%; N 12.60%; O 14.40%

Physical Description: Oil

Boiling Point: Bp_{0.5} 75-80°

References:

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Ried, W. *et al.*, *Annalen*, 1964, **678**, 113, (*synth*)

Reinheckel, H. *et al.*, *Angew. Chem., Int. Ed.*, 1965, **4**, 785; 1966, **5**, 511, (*synth*)

Vita, G. *et al.*, *Chem. Ber.*, 1966, **99**, 3387, (*synth*)

Kawashima, M. *et al.*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 3255, (*synth*)

Coveney, D.J. *et al.*, *J.C.S. Perkin I*, 1990, 2721, (*nitrile*)

Schick, H. *et al.*, *Synthesis*, 1992, 369, (*synth*)