



>>Entry Name: 1,3-Cycloheptanedione, 9CI

CAS Registry Number: 1194-18-9

Structure by analogy with 1,2-Cycloheptanedione, [CXW11-I](#)

Molecular Formula: C₇H₁₀O₂

Molecular Weight: 126.155

Accurate Mass: 126.06808

Percentage Composition: C 66.65%; H 7.99%; O 25.36%

Physical Description: Oil

Boiling Point: Bp₁₅ 119-122°

Refractive Index: n_D^{22.5} 1.4832

>>Derivative: Dioxime

CAS Registry Number: 70820-73-4

Molecular Formula: C₇H₁₂N₂O₂

Molecular Weight: 156.184

Accurate Mass: 156.089878

Percentage Composition: C 53.83%; H 7.74%; N 17.94%; O 20.49%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 162-163°

>>Derivative: Bis-2,4-dinitrophenylhydrazone

Physical Description: Orange cryst. (MeOH)

Melting Point: Mp 205-206°

>>Derivative: Disemicarbazone

Physical Description: Cryst. (EtOH)

Melting Point: Mp 214 dec.°

Solubility: BERDY SOL: Sol. MeOH, Et₂O, H₂O; poorly sol. EtOH, Me₂CO, C₆H₆, CHCl₃

References:

Eistert, B. *et al.*, *Annalen*, 1963, **665**, 55, (*synth*)

Maclean, I. *et al.*, *Tetrahedron*, 1965, **21**, 31, (*synth*)

Hadjarapoglou, L. *et al.*, *Synthesis*, 1996, 525, (*synth*)