



>>Entry Name: **2,3-Octanedione**, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2,3-Dioxooctane. Methyl pentyl diketone

CAS Registry Number: 585-25-1

$\text{H}_3\text{CCOCOCH}_2(\text{CH}_2)_3\text{CH}_3$

Molecular Formula: $\text{C}_8\text{H}_{14}\text{O}_2$

Molecular Weight: 142.197

Accurate Mass: 142.09938

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

Use/Importance: Flavouring material for coffee and tobacco

Physical Description: Liq.

Boiling Point: Bp_{17} 65-67°

>>Derivative: Dioxime

CAS Registry Number: 1844-13-9

Molecular Formula: $\text{C}_8\text{H}_{16}\text{N}_2\text{O}_2$

Molecular Weight: 172.227

Accurate Mass: 172.121178

Percentage Composition: C 55.79%; H 9.36%; N 16.27%; O 18.58%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 173°

>>Derivative: Bis-2,4-dinitrophenylhydrazone

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 221-224°

References:

Jones, L.A. *et al.*, *J.O.C.*, 1961, **26**, 228, (*synth*)

Reusch, W. *et al.*, *Tetrahedron*, 1967, **23**, 2893, (*ms*)

Meister, H. *et al.*, *Annalen*, 1969, **724**, 128, (*synth*)

Venien, F., *C. R. Hebd. Seances Acad. Sci. Ser. C*, 1973, **277**, 247, (*nmr*)

Bowlus, S.B. *et al.*, *J.O.C.*, 1974, **39**, 3309, (*synth, spectra*)