



>>Entry Name: 2,4,4-Trimethyl-2-pentanamine, 9CI

Synonym(s): 1,1,3,3-Tetramethylbutanamine, 8CI. *N*-tert-Octylamine

CAS Registry Number: 107-45-9

Related CAS Registry Numbers(s): 21790-35-2 58618-91-0 68295-35-2

$(\text{H}_3\text{C})_3\text{CCH}_2\text{C}(\text{CH}_3)_2\text{NH}_2$

Molecular Formula: $\text{C}_8\text{H}_{19}\text{N}$

Molecular Weight: 129.245

Accurate Mass: 129.151749

Percentage Composition: C 74.35%; H 14.82%; N 10.84%

Physical Description: Liq.

Boiling Point: Bp 137-143°

Density: d_4^{20} 0.77

Refractive Index: n_D^{20} 1.4240

Aldrich: O-600-0

Fluka: 75000

>>Derivative: Hydrochloride

CAS Registry Number: 58618-91-0

Physical Description: Cryst.

Melting Point: Mp 210°

>>Derivative: *N*-Ac

CAS Registry Number: 5459-42-7

Molecular Formula: $\text{C}_{10}\text{H}_{21}\text{NO}$

Molecular Weight: 171.282

Accurate Mass: 171.162314

Percentage Composition: C 70.12%; H 12.36%; N 8.18%; O 9.34%

Physical Description: Needles (petrol)

Melting Point: Mp 100.5°

>>Derivative: *N*-Benzoyl

CAS Registry Number: 34021-55-1

Molecular Formula: $\text{C}_{15}\text{H}_{23}\text{NO}$

Molecular Weight: 233.353

Accurate Mass: 233.177964

Percentage Composition: C 77.21%; H 9.93%; N 6.00%; O 6.86%

Physical Description: Needles (petrol)

Melting Point: Mp 68.5°

>>Derivative: *N*-(4-Methylbenzenesulfonyl)

CAS Registry Number: 35129-76-1

Molecular Formula: $\text{C}_{15}\text{H}_{25}\text{NO}_2\text{S}$

Molecular Weight: 283.434

Accurate Mass: 283.160599

Percentage Composition: C 63.57%; H 8.89%; N 4.94%; O 11.29%; S 11.31%

Physical Description: Prisms (EtOH)

Melting Point: Mp 134.5-135.5°

References:

Brock, M.J. *et al.*, *Anal. Chem.*, 1955, **27**, 1374-1378, (*cryst struct*)

Whitmore, F.C. *et al.*, *J.A.C.S.*, 1941, **63**, 2035, (*synth, N-Ac*)

Ritter, J.J. *et al.*, *J.A.C.S.*, 1948, **70**, 4045; 4048, (*synth, N-Ac*)

Lacey, R.N., *J.C.S.*, 1960, 1633, (*acyl derivs*)

Oswald, A.A. *et al.*, *J.O.C.*, 1961, **26**, 3969, (*ir*)

Eggert, H. *et al.*, *J.A.C.S.*, 1973, **95**, 3710-3718, (*cmr*)