



>>Entry Name: 7-Aminoheptanoic acid, 9CI

CAS Registry Number: 929-17-9

Related CAS Registry Numbers(s): 5673-25-6

$\text{H}_2\text{NCH}_2(\text{CH}_2)_4\text{CH}_2\text{COOH}$

Molecular Formula: $\text{C}_7\text{H}_{15}\text{NO}_2$

Molecular Weight: 145.201

Accurate Mass: 145.110279

Percentage Composition: C 57.90%; H 10.41%; N 9.65%; O 22.04%

Use/Importance: Used to manuf. nylon-type polymers

Physical Description: Cryst. (H_2O or MeOH/petrol)

Melting Point: Mp 195-196° (186-187°)

pKa Value: $\text{p}K_{\text{a}1}$ 4.5 (25°)

Aldrich: 28463-7

Fluka: 8045

Rare Chemicals Library: S64942-2

Sigma: A9534

>>Derivative: Me ester

CAS Registry Number: 39979-08-3

Molecular Formula: $\text{C}_8\text{H}_{17}\text{NO}_2$

Molecular Weight: 159.228

Accurate Mass: 159.125929

Percentage Composition: C 60.35%; H 10.76%; N 8.80%; O 20.10%

Physical Description: Oil

>>Derivative: Amide

Synonym(s): 7-Aminoheptanamide

CAS Registry Number: 98433-13-7

Molecular Formula: $\text{C}_7\text{H}_{16}\text{N}_2\text{O}$

Molecular Weight: 144.216

Accurate Mass: 144.126263

Percentage Composition: C 58.30%; H 11.18%; N 19.42%; O 11.09%

Physical Description: Cryst. (EtOAc/Et₂O)

Melting Point: Mp 61°

Boiling Point: Bp_{0.3} 145-149°

>>Derivative: N-Et

Molecular Formula: $\text{C}_9\text{H}_{19}\text{NO}_2$

Molecular Weight: 173.255

Accurate Mass: 173.141579

Percentage Composition: C 62.39%; H 11.05%; N 8.08%; O 18.47%

Melting Point: Mp 129-130°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 879A, (*nmr*)

v. Braun, J., *Ber.*, 1907, **40**, 1840; 1909, **42**, 2035, (*synth*)

Novotny, A., *Chem. Listy*, 1958, **52**, 718; *CA*, **52**, 13623, (*synth*)

Berther, C., *Chem. Ber.*, 1959, **92**, 2616, (*amide*)

Japan. Pat., 1975, 75 12 411; *CA*, **83**, 132271n, (*synth*)

Weinkam, R.J., *J.O.C.*, 1978, **43**, 2581, (*ms*)

Petrini, M. *et al.*, *Synthesis*, 1987, 713, (*synth, pmr, esters*)

Ballini, R. *et al.*, *Eur. J. Org. Chem.*, 1999, 87-90, (*synth, ir, pmr*)