



>>Entry Name: Nonafluoropentanoic acid, 9CI

Synonym(s): Perfluoropentanoic acid. Perfluorovaleric acid

CAS Registry Number: 2706-90-3

Related CAS Registry Numbers(s): 336-23-2 2706-89-0 13038-26-1 68259-11-0

$\text{F}_3\text{C}(\text{CF}_2)_3\text{COOH}$

Molecular Formula: $\text{C}_5\text{HF}_9\text{O}_2$

Molecular Weight: 264.047

Accurate Mass: 263.983282

Percentage Composition: C 22.74%; H 0.38%; F 64.76%; O 12.12%

Physical Description: Liq.

Boiling Point: Bp 140° (127°)

Density: d_4^{20} 1.713

Aldrich: 39657-5

Fluka: 77285

>>Derivative: Et ester

CAS Registry Number: 424-36-2

Molecular Formula: $\text{C}_7\text{H}_5\text{F}_9\text{O}_2$

Molecular Weight: 292.101

Accurate Mass: 292.014582

Percentage Composition: C 28.78%; H 1.73%; F 58.54%; O 10.95%

Boiling Point: Bp 121° (105°). Bp₂₀ 65°

>>Derivative: Chloride

CAS Registry Number: 375-60-0

Molecular Formula: $\text{C}_5\text{ClF}_9\text{O}$

Molecular Weight: 282.493

Accurate Mass: 281.949394

Percentage Composition: C 21.26%; Cl 12.55%; F 60.53%; O 5.66%

Boiling Point: Bp 67.5-68°

>>Derivative: Amide

CAS Registry Number: 13485-61-5

Molecular Formula: $\text{C}_5\text{H}_2\text{F}_9\text{NO}$

Molecular Weight: 263.063

Accurate Mass: 262.999266

Percentage Composition: C 22.83%; H 0.77%; F 65.00%; N 5.32%; O 6.08%

Melting Point: Mp 84-85°

Boiling Point: Bp 178-180°

>>Derivative: Nitrile

Synonym(s): 1-Cyano-2,2,3,3,4,4,5,5,5-nonafluorobutane

CAS Registry Number: 22325-71-9

Molecular Formula: $\text{C}_3\text{F}_9\text{N}$

Molecular Weight: 245.047

Accurate Mass: 244.988701

Percentage Composition: C 24.51%; F 69.78%; N 5.72%

Boiling Point: Bp *ca.* ° 15

References:

Kauck, E.A. *et al.*, *Ind. Eng. Chem.*, 1951, **43**, 2332; *CA*, **46**, 4478f, (*synth*)

Simons, J.H. *et al.*, *J.A.C.S.*, 1953, **75**, 5621, (*chloride*)

Hazeldine, R.N. *et al.*, *J.C.S.*, 1956, 61, (*synth*)

Thoai, N. *et al.*, *J. Fluorine Chem.*, 1982, **20**, 271, (*ester, nitrile*)

Bénéfice, S. *et al.*, *Tetrahedron*, 1984, **40**, 1541-1544, (*synth, ir, F-19 nmr, ms*)

Bénéfice-Malouet, S. *et al.*, *Synthesis*, 1991, 647, (*synth, pmr, F-19 nmr, ms*)