



>>Entry Name: Heptadecafluorononanoic acid, 9Cl, 8Cl

Synonym(s): Perfluorononanoic acid

CAS Registry Number: 375-95-1

Related CAS Registry Numbers(s): 558-95-2 4149-60-4 21049-38-7 21049-39-8 55795-92-1 82854-34-0 117374-38-6

$\text{F}_3\text{C}(\text{CF}_2)_7\text{COOH}$

Molecular Formula: $\text{C}_9\text{HF}_{17}\text{O}_2$

Molecular Weight: 464.079

Accurate Mass: 463.970506

Percentage Composition: C 23.29%; H 0.22%; F 69.59%; O 6.90%

Physical Description: Cryst. (CCl_4)

Melting Point: Mp 69-71° (65°)

Aldrich: 39445-9

Fluka: 77284

>>Derivative: Me ester

CAS Registry Number: 51502-45-5

Molecular Formula: $\text{C}_{10}\text{H}_3\text{F}_{17}\text{O}_2$

Molecular Weight: 478.105

Accurate Mass: 477.986156

Percentage Composition: C 25.12%; H 0.63%; F 67.55%; O 6.69%

Boiling Point: Bp₂₁ 78.2-79.5°

Other: OAKWOOD: 2279

>>Derivative: Et ester

CAS Registry Number: 30377-52-7

Molecular Formula: $\text{C}_{11}\text{H}_5\text{F}_{17}\text{O}_2$

Molecular Weight: 492.132

Accurate Mass: 492.001806

Percentage Composition: C 26.85%; H 1.02%; F 65.63%; O 6.50%

Boiling Point: Bp 200°. Bp₂₀ 105°. Bp₁₈ 82-83.5°

>>Derivative: Chloride

CAS Registry Number: 52447-23-1

Molecular Formula: $\text{C}_9\text{ClF}_{17}\text{O}$

Molecular Weight: 482.524

Accurate Mass: 481.936618

Percentage Composition: C 22.40%; Cl 7.35%; F 66.93%; O 3.32%

Physical Description: Liq.

>>Derivative: Nitrile

Synonym(s): Heptadecafluorononanenitrile

CAS Registry Number: 82416-71-5

Molecular Formula: $\text{C}_9\text{F}_{17}\text{N}$

Molecular Weight: 445.079

Accurate Mass: 444.975925

Percentage Composition: C 24.29%; F 72.57%; N 3.15%

Boiling Point: Bp 115°

References:

- Smith, C.F. *et al.*, *J. Fluorine Chem.*, 1974, **4**, 35, (ester, F-19 nmr, ms)
Blancou, H. *et al.*, *Chem. Comm.*, 1976, 885, (synth)
Thoai, N. *et al.*, *J. Fluorine Chem.*, 1982, **20**, 271, (nitrile)
Ishikawa, N. *et al.*, *J. Fluorine Chem.*, 1983, **22**, 585, (synth)
Benefice, S. *et al.*, *Tetrahedron*, 1984, **40**, 1541, (synth, Raman, ester)
Afzal, J. *et al.*, *J. Fluorine Chem.*, 1986, **34**, 385, (synth)
Troemel, M. *et al.*, *Angew. Chem., Int. Ed.*, 1987, **26**, 1007, (synth)
Eur. Pat., 1988, 271 212; *CA*, **109**, 210556f, (esters)
Benefice-Malouet, S. *et al.*, *Synthesis*, 1991, 647, (synth, pmr, F-19 nmr)