



>>Entry Name: Heptafluorobutanoic acid, 9CI

Synonym(s): Perfluorobutyric acid

CAS Registry Number: 375-22-4

F3CCF2CF2COOH

Molecular Formula: C4HF7O2

Molecular Weight: 214.039

Accurate Mass: 213.986476

Percentage Composition: C 22.45%; H 0.47%; F 62.13%; O 14.95%

Physical Description: Liq.

Melting Point: Mp  $-19.9^{\circ}$

Boiling Point: Bp  $120.8-121^{\circ}$

Solubility: Sol. H2O, Et2O, toluene

Density:  $d_4^{20}$  1.65

Refractive Index:  $n_D^{25}$  1.2950

Hazard & Toxicity: LD<sub>50</sub> (mus, ipr) 153 mg/kg

Aldrich: 16419-4

Fluka: 77249

Sigma: H7133

>>Derivative: Me ester

CAS Registry Number: 356-24-1

Molecular Formula: C5H3F7O2

Molecular Weight: 228.066

Accurate Mass: 228.002126

Percentage Composition: C 26.33%; H 1.33%; F 58.31%; O 14.03%

Physical Description: Liq.

Melting Point: Mp  $-86^{\circ}$

Boiling Point: Bp  $81.5-82^{\circ}$

Solubility: Sl. sol. H2O; sol. Et2O, Me2CO

Density:  $d^{20}$  1.483

Refractive Index:  $n_D^{20}$  1.2950

Aldrich: 28229-4

Sigma: H2014

>>Derivative: Et ester

CAS Registry Number: 356-27-4

Molecular Formula: C6H5F7O2

Molecular Weight: 242.093

Accurate Mass: 242.017776

Percentage Composition: C 29.77%; H 2.08%; F 54.93%; O 13.22%

Physical Description: Liq.

Boiling Point: Bp  $96.6^{\circ}$

Solubility: Sl. sol. H2O; sol. Et2O, Me2CO

Density:  $d^{20}$  1.394

Refractive Index:  $n_D^{20}$  1.3011

Hazard & Toxicity: LD<sub>50</sub> (rbt, ipr) 250 mg/kg

Aldrich: 17514-5

Fluka: 77258

>>Derivative: Vinyl ester

CAS Registry Number: 356-28-5

Molecular Formula: C6H3F7O2

Molecular Weight: 240.077

Accurate Mass: 240.002126

Percentage Composition: C 30.02%; H 1.26%; F 55.39%; O 13.33%

Physical Description: Liq.

Boiling Point: Bp<sub>745</sub>  $78-79^{\circ}$

Refractive Index:  $n_D^{20}$  1.3086

Other Data: Undergoes radical polym. Q/e values for copolym., Q 0.024, e  $-0.89$