



>>Entry Name: Fluoropropanedioic acid, 9CI

Synonym(s): Fluoromalonic acid

CAS Registry Number: 473-87-0

Related CAS Registry Numbers(s): 3107-39-9

HOOCCHF₂COOH

Molecular Formula: C₃H₃FO₄

Molecular Weight: 122.053

Accurate Mass: 122.001538

Percentage Composition: C 29.52%; H 2.48%; F 15.57%; O 52.43%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 135.8-136.5°

>>Derivative: Hemi-K salt

CAS Registry Number: 80621-11-0

Physical Description: Cryst. + 1H₂O

Melting Point: Mp 180 dec.°

Hazard & Toxicity: LD₅₀ (rat, scu) 60 mg/kg

>>Derivative: Mono-Et ester (R-)

CAS Registry Number: 94721-39-8

Molecular Formula: C₅H₇FO₄

Molecular Weight: 150.106

Accurate Mass: 150.032838

Percentage Composition: C 40.01%; H 4.70%; F 12.66%; O 42.63%

Physical Description: Liq.

Boiling Point: Bp_{0.4} 103-106°

Optical Rotation: [α]_D +13.9 (c, 2.12 in MeOH) (>99% ee)

>>Derivative: Di-Me ester

CAS Registry Number: 344-14-9

Molecular Formula: C₅H₇FO₄

Molecular Weight: 150.106

Accurate Mass: 150.032838

Percentage Composition: C 40.01%; H 4.70%; F 12.66%; O 42.63%

Physical Description: Liq.

Boiling Point: Bp₄₅ 111-112°. Bp₁₅ 82-85°

>>Derivative: Di-Et ester

CAS Registry Number: 685-88-1

Molecular Formula: C₇H₁₁FO₄

Molecular Weight: 178.16

Accurate Mass: 178.064138

Percentage Composition: C 47.19%; H 6.22%; F 10.66%; O 35.92%

Physical Description: Liq.

Boiling Point: Bp₂₀ 110-111°. Bp₁₂ 94-96°

Hazard & Toxicity: LD₅₀ (rat, scu) 70 mg/kg

Aldrich: 28558-7

Fluka: 47105

Sigma: D8634

>>Derivative: Dibenzyl ester

CAS Registry Number: 133384-81-3

Molecular Formula: C₁₇H₁₅FO₄

Molecular Weight: 302.301

Accurate Mass: 302.095438

Percentage Composition: C 67.54%; H 5.00%; F 6.28%; O 21.17%

Melting Point: Mp 52-53°