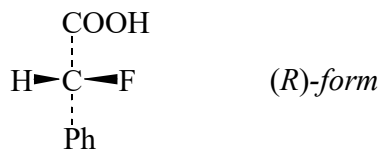




>>Entry Name: Fluorophenylacetic acid

Synonym(s): α -Fluorobenzeneacetic acid, 9CI



Molecular Formula: C₈H₇FO₂

Molecular Weight: 154.14

Accurate Mass: 154.043008

Percentage Composition: C 62.34%; H 4.58%; F 12.33%; O 20.76%

>>Variant: (R)-form

CAS Registry Number: 63818-94-0

Molecular Formula: C₈H₇FO₂

Molecular Weight: 154.14

Accurate Mass: 154.043008

Percentage Composition: C 62.34%; H 4.58%; F 12.33%; O 20.76%

Physical Description: Needles (hexane/Et₂O)

Melting Point: Mp 103-105°

Optical Rotation: [α]_D²³ -153.5 (c, 1.52 in Me₂CO)

>>Variant: (S)-form

CAS Registry Number: 63818-95-1

Molecular Formula: C₈H₇FO₂

Molecular Weight: 154.14

Accurate Mass: 154.043008

Percentage Composition: C 62.34%; H 4.58%; F 12.33%; O 20.76%

Physical Description: Cryst.

Melting Point: Mp 99-101°

Optical Rotation: [α]_D²³ +136.5 (c, 1.45 in Me₂CO)

>>Variant: (±)-form

CAS Registry Number: 1578-63-8

Molecular Formula: C₈H₇FO₂

Molecular Weight: 154.14

Accurate Mass: 154.043008

Percentage Composition: C 62.34%; H 4.58%; F 12.33%; O 20.76%

Physical Description: Cryst. (petrol/C₆H₆)

Melting Point: Mp 83-85°

Boiling Point: Bp_{0.1} 65-68° subl.

Aldrich: 21952-5

Sigma: F6254

>>Derivative: K salt

CAS Registry Number: 22692-91-7

Melting Point: Mp 218-220°

>>Derivative: Me ester

CAS Registry Number: 17841-30-4

Molecular Formula: C₉H₉FO₂

Molecular Weight: 168.167

Accurate Mass: 168.058658

Percentage Composition: C 64.28%; H 5.39%; F 11.30%; O 19.03%

Boiling Point: Bp₂₄ 126-131°