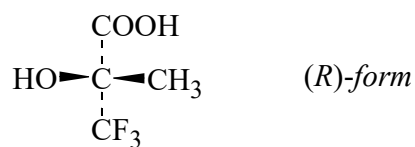




>>Entry Name: 3,3,3-Trifluoro-2-hydroxy-2-methylpropanoic acid, 9CI

Synonym(s): 3,3,3-Trifluoro-2-methylactic acid, 8CI



CAS Registry Number: 374-35-6

Related CAS Registry Numbers(s): 337-16-6 161343-81-3

Molecular Formula: C₄H₅F₃O₃

Molecular Weight: 158.077

Accurate Mass: 158.019079

Percentage Composition: C 30.39%; H 3.19%; F 36.06%; O 30.36%

>>Variant: (*R*)-form

CAS Registry Number: 44864-47-3

Molecular Formula: C₄H₅F₃O₃

Molecular Weight: 158.077

Accurate Mass: 158.019079

Percentage Composition: C 30.39%; H 3.19%; F 36.06%; O 30.36%

Melting Point: Mp 106-110°

Optical Rotation: [α]_D²²+18.4 (c, 2.55 in MeOH) (>99% ee)

>>Derivative: Me ether

Synonym(s): 3,3,3-Trifluoro-2-methoxy-2-methylpropanoic acid

CAS Registry Number: 166584-04-9

Molecular Formula: C₅H₇F₃O₃

Molecular Weight: 172.104

Accurate Mass: 172.034729

Percentage Composition: C 34.89%; H 4.10%; F 33.12%; O 27.89%

Boiling Point: Bp₂₄ 95°

Optical Rotation: [α]_D²⁰−4.31 (neat)

>>Variant: (*S*)-form

CAS Registry Number: 24435-45-8

Molecular Formula: C₄H₅F₃O₃

Molecular Weight: 158.077

Accurate Mass: 158.019079

Percentage Composition: C 30.39%; H 3.19%; F 36.06%; O 30.36%

Physical Description: Solid

Melting Point: Mp 105-108°

Optical Rotation: [α]_D²³−18.9 (c, 9.04 in MeOH)

>>Derivative: Me ether

CAS Registry Number: 139714-79-7

Molecular Formula: C₅H₇F₃O₃

Molecular Weight: 172.104

Accurate Mass: 172.034729

Percentage Composition: C 34.89%; H 4.10%; F 33.12%; O 27.89%

Use/Importance: Amino acid derivatising agent for low temperature gc resolution

Boiling Point: Bp₁₈ 93°

Optical Rotation: [α]_D²⁰+4.3 (neat)

Density: d₄¹⁸ 1.32