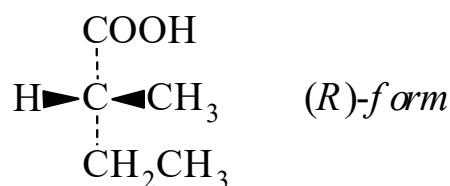




>>Entry Name: 2-Methylbutanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Ethylmethylacetic acid. Butane-2-carboxylic acid. FEMA 2695



CAS Registry Number: 116-53-0

Related CAS Registry Numbers(s): 868-57-5 86491-60-3

Molecular Formula: C₅H₁₀O₂

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

Aldrich: 19307-0

>>Variant: (R)-form

CAS Registry Number: 32231-50-8

Molecular Formula: C₅H₁₀O₂

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

Biological Source: Degradn. prod. of many natural products

Boiling Point: Bp 176-177°

Optical Rotation: $[\alpha]_{\text{D}}^{28} -18.7$ (c, 0.76 in EtOH)

>>Derivative: Me ester

CAS Registry Number: 55449-44-0

Molecular Formula: C₆H₁₂O₂

Molecular Weight: 116.16

Accurate Mass: 116.08373

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Boiling Point: Bp 115-116°

Optical Rotation: $[\alpha]_{\text{D}}^{15} -19.42$ (H₂O)

>>Variant: (S)-form

CAS Registry Number: 1730-91-2

Molecular Formula: C₅H₁₀O₂

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

Biological Source: Isol. from many essential oils and other biol. sources

Boiling Point: Bp 177°. Bp₁₅ 76-78°

Aldrich: 24552-6

Fluka: 66127

Sigma: M0516

>>Derivative: Me ester

CAS Registry Number: 10307-60-5

Molecular Formula: C₆H₁₂O₂

Molecular Weight: 116.16

Accurate Mass: 116.08373

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Biological Source: Flavour component of apple and strawberry

Boiling Point: Bp 115.5-116°

Optical Rotation: $[\alpha]_{\text{D}} +16.56$ (H₂O)