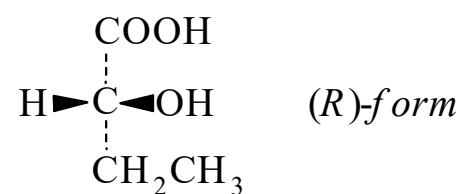




>>Entry Name: 2-Hydroxybutanoic acid, 9CI



CAS Registry Number: 565-70-8

Related CAS Registry Numbers(s): 4476-02-2 19947-43-4 35054-79-6 52089-54-0 54839-26-8

Molecular Formula: C₄H₈O₃

Molecular Weight: 104.105

Accurate Mass: 104.047345

Percentage Composition: C 46.15%; H 7.75%; O 46.11%

Source/Synthesis: Present in tobacco smoke

>>Variant: (R)-form

CAS Registry Number: 20016-85-7

Molecular Formula: C₄H₈O₃

Molecular Weight: 104.105

Accurate Mass: 104.047345

Percentage Composition: C 46.15%; H 7.75%; O 46.11%

Optical Rotation: $[\alpha]_{\text{D}}^{25} +6$ (H₂O)

>>Derivative: Me ester

CAS Registry Number: 73349-07-2

Molecular Formula: C₅H₁₀O₃

Molecular Weight: 118.132

Accurate Mass: 118.062995

Percentage Composition: C 50.84%; H 8.53%; O 40.63%

Boiling Point: Bp₃₃ 73-75°

Optical Rotation: $[\alpha]_{\text{D}}^{21} +5.12$ (neat)

>>Derivative: Et ester

CAS Registry Number: 87172-81-4

Molecular Formula: C₆H₁₂O₃

Molecular Weight: 132.159

Accurate Mass: 132.078645

Percentage Composition: C 54.53%; H 9.15%; O 36.32%

Boiling Point: Bp₂₀ 80-81°

Optical Rotation: $[\alpha]_{\text{D}}^{22} +8.4$ (neat). $[\alpha]_{\text{D}}^{20} -13.8$ (c, 10 in EtOH)

>>Derivative: Me ether

CAS Registry Number: 54623-60-8

Molecular Formula: C₅H₁₀O₃

Molecular Weight: 118.132

Accurate Mass: 118.062995

Percentage Composition: C 50.84%; H 8.53%; O 40.63%

Optical Rotation: $[\alpha]_{\text{D}}^{25} -77.6$ (neat)

>>Variant: (S)-form

Synonym(s): L_S-form (obsol.)

CAS Registry Number: 3347-90-8

Molecular Formula: C₄H₈O₃

Molecular Weight: 104.105

Accurate Mass: 104.047345

Percentage Composition: C 46.15%; H 7.75%; O 46.11%

Physical Description: Needles (CCl₄/hexane)

Melting Point: Mp 55-55.5° (52.5-53.5°)

Optical Rotation: $[\alpha]_{\text{D}}^{16} -3$ (c, 6.19 in H₂O). $[\alpha]_{\text{D}}^{16} +6.4$ (c, 11.03 in CHCl₃). $[\alpha]_{\text{D}}^{25} -6.8$ (H₂O)

Other Data: The opt. rotn. is extremely variable with solv. and concn. and should not be used as a criterion of config. or purity