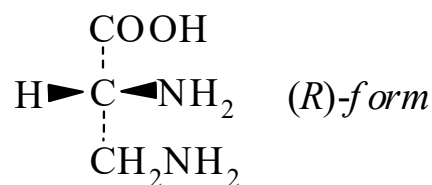




>>Entry Name: **2,3-Diaminopropanoic acid**

Synonym(s): 3-Aminoalanine, 9CI



CAS Registry Number: 515-94-6

Related CAS Registry Numbers(s): 1482-97-9 6018-55-9 61049-68-1 69531-11-9

Molecular Formula: $\text{C}_3\text{H}_8\text{N}_2\text{O}_2$

Molecular Weight: 104.108

Accurate Mass: 104.058578

Percentage Composition: C 34.61%; H 7.75%; N 26.91%; O 30.74%

>>Variant: (R)-form

Synonym(s): D-form

Molecular Formula: $\text{C}_3\text{H}_8\text{N}_2\text{O}_2$

Molecular Weight: 104.108

Accurate Mass: 104.058578

Percentage Composition: C 34.61%; H 7.75%; N 26.91%; O 30.74%

>>Derivative: Hydrochloride (1:2)

Optical Rotation: $[\alpha]_{\text{D}}^{25} -25.2$ (1N HCl)

>>Derivative: N,N'-Dibenzoyl

Molecular Formula: $\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_4$

Molecular Weight: 312.324

Accurate Mass: 312.111008

Percentage Composition: C 65.38%; H 5.16%; N 8.97%; O 20.49%

Melting Point: Mp 156-157°

Optical Rotation: $[\alpha]_{\text{D}}^{16} -23.9$ (MeOH)

>>Derivative: N,N'-Dibenzoyl, Me ester

Molecular Formula: $\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_4$

Molecular Weight: 326.351

Accurate Mass: 326.126658

Percentage Composition: C 66.25%; H 5.56%; N 8.58%; O 19.61%

Melting Point: Mp 153-154°

Optical Rotation: $[\alpha]_{\text{D}}^{16} -21.58$ (MeOH)

>>Derivative: N,N'-Dibenzoyl, Et ester

Molecular Formula: $\text{C}_{19}\text{H}_{20}\text{N}_2\text{O}_4$

Molecular Weight: 340.378

Accurate Mass: 340.142308

Percentage Composition: C 67.05%; H 5.92%; N 8.23%; O 18.80%

Melting Point: Mp 151°

Optical Rotation: $[\alpha]_{\text{D}}^{18} -13.3$ (EtOH)

>>Derivative: N³-Me

CAS Registry Number: 20790-80-1

Molecular Formula: $\text{C}_4\text{H}_{10}\text{N}_2\text{O}_2$

Molecular Weight: 118.135

Accurate Mass: 118.074228

Percentage Composition: C 40.67%; H 8.53%; N 23.71%; O 27.09%

Melting Point: Mp 168°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -35$ (c, 1.2 in 5M HCl)