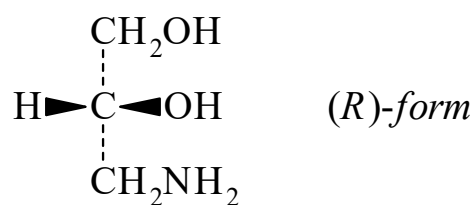




>>Entry Name: 3-Amino-1,2-propanediol, 9CI

Synonym(s): 2,3-Dihydroxypropylamine. 3-Aminopropylene glycol



CAS Registry Number: 616-30-8

Related CAS Registry Numbers(s): 60812-23-9

Molecular Formula: $\text{C}_3\text{H}_9\text{NO}_2$

Molecular Weight: 91.11

Accurate Mass: 91.063329

Percentage Composition: C 39.55%; H 9.96%; N 15.37%; O 35.12%

Aldrich: A7600-1

Fluka: 9265

Sigma: A9161

>>Variant: (R)-form

Molecular Formula: $\text{C}_3\text{H}_9\text{NO}_2$

Molecular Weight: 91.11

Accurate Mass: 91.063329

Percentage Composition: C 39.55%; H 9.96%; N 15.37%; O 35.12%

Boiling Point: Bp_{15} 163°

Optical Rotation: $[\alpha]_{\text{D}}^{18} +2.4$ (H_2O) (dil. HCl)

>>Variant: (S)-form

Molecular Formula: $\text{C}_3\text{H}_9\text{NO}_2$

Molecular Weight: 91.11

Accurate Mass: 91.063329

Percentage Composition: C 39.55%; H 9.96%; N 15.37%; O 35.12%

Melting Point: Mp 55-57°

Boiling Point: $\text{Bp}_{0.003}$ 95-98°

Optical Rotation: $[\alpha]_{\text{D}} -2.4$ (H_2O) (dil. HCl)

>>Variant: (±)-form

Molecular Formula: $\text{C}_3\text{H}_9\text{NO}_2$

Molecular Weight: 91.11

Accurate Mass: 91.063329

Percentage Composition: C 39.55%; H 9.96%; N 15.37%; O 35.12%

Boiling Point: Bp 264-265° (part dec.). $\text{Bp}_{1.5}$ 110-115° (lit. gives a pressure range)

Other Data: Hygroscopic, absorbs CO_2

>>Derivative: O,O-Dibenzoyl

Molecular Formula: $\text{C}_{17}\text{H}_{17}\text{NO}_4$

Molecular Weight: 299.326

Accurate Mass: 299.115759

Percentage Composition: C 68.22%; H 5.72%; N 4.68%; O 21.38%

Physical Description: Needles (as hydrochloride)

Melting Point: Mp 203 dec.° (hydrochloride)

>>Derivative: Tribenzoyl

Molecular Formula: $\text{C}_{24}\text{H}_{21}\text{NO}_5$

Molecular Weight: 403.434

Accurate Mass: 403.141974

Percentage Composition: C 71.45%; H 5.25%; N 3.47%; O 19.83%

Melting Point: Mp 113-114°