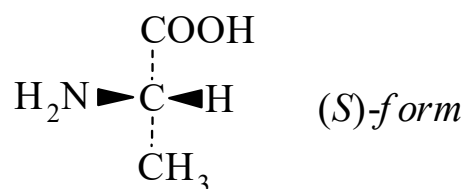




>>Entry Name: Alanine, INN, USAN

Synonym(s): 2-Aminopropanoic acid, 9CI.  $\alpha$ -Alanine. Ala



Related CAS Registry Numbers(s): 2134-48-7 2491-20-5 3082-75-5 17831-01-5 33208-99-0 34404-37-0 95596-57-9 98204-12-7

Molecular Formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>

Molecular Weight: 89.094

Accurate Mass: 89.047679

Percentage Composition: C 40.44%; H 7.92%; N 15.72%; O 35.92%

>>Variant: (*R*)-form

Synonym(s): D-form

CAS Registry Number: 338-69-2

Molecular Formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>

Molecular Weight: 89.094

Accurate Mass: 89.047679

Percentage Composition: C 40.44%; H 7.92%; N 15.72%; O 35.92%

Biological Source: Occurs in the cell walls of bacteria and in some higher plants

Physical Description: Prisms (EtOH aq.)

Melting Point: Mp 295-297 dec.°

Optical Rotation:  $[\alpha]_{\text{D}}^{25} -1.8$  (c, 1 in H<sub>2</sub>O).  $[\alpha]_{\text{D}} -14.6$  (c, 1 in 5*M* HCl)

Solubility: Sol. hot H<sub>2</sub>O

Aldrich: 16265-5

Fluka: 5140

Sigma: A7377

>>Derivative: Hydrochloride

Optical Rotation:  $[\alpha]_{\text{D}}^{20} -10.3$  (H<sub>2</sub>O)

Solubility: Sol. H<sub>2</sub>O

>>Derivative: Me ester

CAS Registry Number: 21705-13-5

Extra CAS Registry Numbers(s): 14316-06-4

Molecular Formula: C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>

Molecular Weight: 103.121

Accurate Mass: 103.063329

Percentage Composition: C 46.59%; H 8.80%; N 13.58%; O 31.03%

Melting Point: Mp 109-111° (as hydrochloride)

>>Derivative: Et ester

CAS Registry Number: 30959-96-7

Molecular Formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>

Molecular Weight: 117.147

Accurate Mass: 117.078979

Percentage Composition: C 51.26%; H 9.46%; N 11.96%; O 27.31%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 104-105°

Optical Rotation:  $[\alpha]_{\text{D}}^{20} +6.91$  (EtOH)

>>Derivative: Benzyl ester

CAS Registry Number: 17831-02-6

Molecular Formula: C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub>

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Melting Point: Mp 139-140° (as hydrochloride)

Optical Rotation:  $[\alpha]_{\text{D}}^{25} +10.5$  (c, 2 in 0.1*M* HCl)