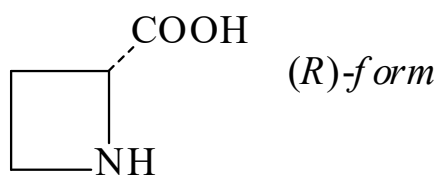




>>Entry Name: 2-Azetidinecarboxylic acid, 9CI



CAS Registry Number: 2517-04-6

Molecular Formula: $C_4H_7NO_2$

Molecular Weight: 101.105

Accurate Mass: 101.047679

Percentage Composition: C 47.52%; H 6.98%; N 13.85%; O 31.65%

>>Variant: (R)-form

CAS Registry Number: 7729-30-8

Molecular Formula: $C_4H_7NO_2$

Molecular Weight: 101.105

Accurate Mass: 101.047679

Percentage Composition: C 47.52%; H 6.98%; N 13.85%; O 31.65%

Optical Rotation: $[\alpha]_D^{20} +102$ (c, 3.6 in H_2O)

>>Variant: (S)-form

CAS Registry Number: 2133-34-8

Molecular Formula: $C_4H_7NO_2$

Molecular Weight: 101.105

Accurate Mass: 101.047679

Percentage Composition: C 47.52%; H 6.98%; N 13.85%; O 31.65%

Biological Source: Present in roots and leaves of *Convallaria majalis* (lily-of-the-valley) and other liliaceous plants and seeds of *Fritillaria meleagris*

Use/Importance: Seedling growth inhibitor. Proline antagonist

Physical Description: Cryst. (MeOH)

Optical Rotation: $[\alpha]_D^{20} -108$ (c, 3.6 in H_2O)

Solubility: Sol. H_2O

UV: [neutral] λ_{max} 0 (end) (ϵ) (H_2O) (Derep)

Other Data: Unstable in mineral acids. Does not melt but darkens at 270°

Hazard & Toxicity: Exp. reprod. and teratogenic effects ; BERDY HAZD : LD₅₀ (mus, scu) 1000 mg/kg

Aldrich: A9630-4

Fluka: 11542

Sigma: A0760

>>Derivative: Me ester

CAS Registry Number: 69684-70-4

Molecular Formula: $C_5H_9NO_2$

Molecular Weight: 115.132

Accurate Mass: 115.063329

Percentage Composition: C 52.16%; H 7.88%; N 12.17%; O 27.79%

Physical Description: Cryst. (Et_2O/CH_2Cl_2) (as hydrochloride)

Optical Rotation: $[\alpha]_D -86.8$ (c, 0.5 in H_2O) (hydrochloride)

>>Derivative: Amide

Molecular Formula: $C_4H_8N_2O$

Molecular Weight: 100.12

Accurate Mass: 100.063663

Percentage Composition: C 47.99%; H 8.05%; N 27.98%; O 15.98%

Physical Description: Cryst. ($CH_2Cl_2/EtOAc$)

Melting Point: Mp $114-116^\circ$

Optical Rotation: $[\alpha]_D^{28} -182.9$ (c, 1.007 in $CHCl_3$)