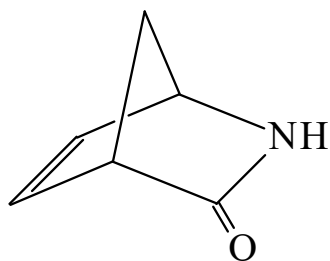




>>Entry Name: 2-Azabicyclo[2.2.1]hept-5-en-3-one, 9Cl

Synonym(s): 4-Amino-2-cyclopentene-1-carboxylic acid lactam. Vince's lactam



(+)-form

CAS Registry Number: 49805-30-3

Molecular Formula: C₆H₇NO

Molecular Weight: 109.127

Accurate Mass: 109.052764

Percentage Composition: C 66.04%; H 6.47%; N 12.84%; O 14.66%

Use/Importance: Important synthon for carbocyclic nucleosides

Aldrich: 33191-0

Fluka: 11374

>>Variant: (+)-form

CAS Registry Number: 130931-83-8

Molecular Formula: C₆H₇NO

Molecular Weight: 109.127

Accurate Mass: 109.052764

Percentage Composition: C 66.04%; H 6.47%; N 12.84%; O 14.66%

Melting Point: Mp 95°

Optical Rotation: $[\alpha]_D^{25} +555$ (>98% ee)

Other Data: Crystallises as a conglomerate

Aldrich: 44128-7

Other: Chiroscience

>>Variant: (–)-form

CAS Registry Number: 79200-56-9

Molecular Formula: C₆H₇NO

Molecular Weight: 109.127

Accurate Mass: 109.052764

Percentage Composition: C 66.04%; H 6.47%; N 12.84%; O 14.66%

Melting Point: Mp 93-95° (86-88°)

Optical Rotation: $[\alpha]_D -556$ (c, 1.1 in CHCl₃)

Aldrich: 44127-9

Other: Chiroscience

>>Variant: (±)-form

CAS Registry Number: 61865-48-3

Molecular Formula: C₆H₇NO

Molecular Weight: 109.127

Accurate Mass: 109.052764

Percentage Composition: C 66.04%; H 6.47%; N 12.84%; O 14.66%

Melting Point: Mp 56°

Boiling Point: Bp_{0.05} 120°

Other Data: Can be resolved on a large scale by spontaneous resolu.

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 1252A, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 786C, (*ir*)
Jagt, J.C. *et al.*, *J.O.C.*, 1974, **39**, 564, (*synth*)
Daluge, S. *et al.*, *J.O.C.*, 1978, **43**, 2311, (*synth*)
Heesing, A. *et al.*, *Chem. Ber.*, 1983, **116**, 1081, (*synth*)
Taylor, S.J.C. *et al.*, *Chem. Comm.*, 1990, 1120, (*resoln*)
Griffiths, G.J. *et al.*, *J.O.C.*, 1993, **58**, 6129, (*synth*, *ir*, *pmr*, *bibl*)
Nakano, H. *et al.*, *Tetrahedron: Asymmetry*, 1994, **5**, 1155, (*synth*)
Potter, G.A. *et al.*, *Angew. Chem., Int. Ed.*, 1996, **35**, 1666-1668, (*resoln*)
Suchod, B. *et al.*, *Acta Cryst. C*, 1997, **53**, 1911-1912, (*(-)-form*, *cryst struct*)