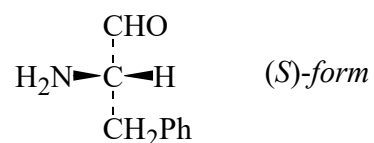




>>Entry Name: 2-Amino-3-phenylpropanal

Synonym(s): α -Aminobenzenepropanal, 9Cl. Phenylalaninal



Molecular Formula: C₉H₁₁NO

Molecular Weight: 149.192

Accurate Mass: 149.084064

Percentage Composition: C 72.46%; H 7.43%; N 9.39%; O 10.72%

>>Variant: (S)-form

CAS Registry Number: 59867-93-5

Molecular Formula: C₉H₁₁NO

Molecular Weight: 149.192

Accurate Mass: 149.084064

Percentage Composition: C 72.46%; H 7.43%; N 9.39%; O 10.72%

Physical Description: No phys. props. reported

>>Derivative: *N,N*-Dibenzyl

CAS Registry Number: 111060-64-1

Molecular Formula: C₂₃H₂₃NO

Molecular Weight: 329.441

Accurate Mass: 329.177964

Percentage Composition: C 83.86%; H 7.04%; N 4.25%; O 4.86%

Physical Description: Oil

Optical Rotation: [α]_D²⁵ -99.4 (c, 1 in CHCl₃)

Other Data: Stable for several weeks when stored at -10° under N₂

Aldrich: 45823-6

>>Derivative: *N-tert*-Butyloxycarbonyl

CAS Registry Number: 72155-45-4

Extra CAS Registry Numbers(s): 77119-85-8

Molecular Formula: C₁₄H₁₉NO₃

Molecular Weight: 249.309

Accurate Mass: 249.136494

Percentage Composition: C 67.45%; H 7.68%; N 5.62%; O 19.25%

Melting Point: Mp 163-164° (as 2,4-dinitrophenylhydrazone)

Optical Rotation: [α]_D²⁰ +2.9 (c, 3.0 in CH₂Cl₂)

References:

- Stanfield, C.F. *et al.*, *J.O.C.*, 1981, **46**, 4797-4798, (*S*-form, ester, synth, pmr, ir)
Fehrentz, J.-A. *et al.*, *Synthesis*, 1983, 676-678, (*S*-form, ester, synth, pmr, ir)
McNulty, J. *et al.*, *Synth. Commun.*, 1992, **22**, 979-985, (*S*-form, ester, synth)
Beaulieu, P.L. *et al.*, *J.O.C.*, 1996, **61**, 3635-3645, (*N,N*-dibenzyl, synth, ir, pmr, cmr)
Dondoni, A. *et al.*, *Synthesis*, 1996, 641-646, (*R*-form, ester, synth, pmr, cmr)
Reetz, M.T., *Chem. Rev.*, 1999, **99**, 1121-1162, (*N,N*-dibenzyl, rev)
Org. Synth., 1999, **76**, 110-122, (*N,N*-dibenzyl, synth, pmr, cmr)