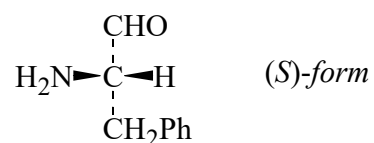




>>Entry Name: 2-Amino-3-phenylpropanal

Synonym(s):  $\alpha$ -Aminobenzenepropanal, 9Cl. Phenylalaninal



**Molecular Formula:** C<sub>9</sub>H<sub>11</sub>NO

**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:** C<sub>9</sub>H<sub>11</sub>NO

**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:** C<sub>23</sub>H<sub>23</sub>NO

**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:**  $[\alpha]_{\text{D}}^{25} -99.4$  (c, 1 in CHCl<sub>3</sub>)

**Other Data:** Stable for several weeks when stored at -10° under N<sub>2</sub>

**Aldrich:** 45823-6

>>Derivative: *N-tert*-Butyloxycarbonyl

**CAS Registry Number:** 72155-45-4

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

**Molecular Formula:** C<sub>14</sub>H<sub>19</sub>NO<sub>3</sub>

**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:**  $[\alpha]_{\text{D}}^{20} +2.9$  (c, 3.0 in CH<sub>2</sub>Cl<sub>2</sub>)

**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)