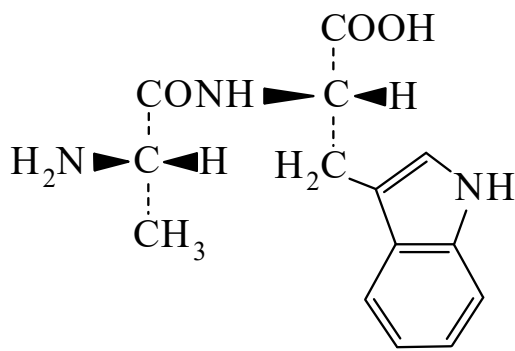




>>Entry Name: *N*-Alanyltryptophan



**Molecular Formula:** C<sub>14</sub>H<sub>17</sub>N<sub>3</sub>O<sub>3</sub>

**Molecular Weight:** 275.307

**Accurate Mass:** 275.126992

**Percentage Composition:** C 61.08%; H 6.22%; N 15.26%; O 17.43%

>>Variant: L-L-form

**CAS Registry Number:** 16305-75-2

**Molecular Formula:** C<sub>14</sub>H<sub>17</sub>N<sub>3</sub>O<sub>3</sub>

**Molecular Weight:** 275.307

**Accurate Mass:** 275.126992

**Percentage Composition:** C 61.08%; H 6.22%; N 15.26%; O 17.43%

**Physical Description:** Cryst. (EtOH/EtOAc)

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>25</sup> +19 (c, 1 in H<sub>2</sub>O)

**Fluka:** 5400

**Sigma:** A3878

>>Derivative: *N*-*tert*-Butyloxycarbonyl, Me ester

**CAS Registry Number:** 207349-24-4

**Molecular Formula:** C<sub>20</sub>H<sub>27</sub>N<sub>3</sub>O<sub>5</sub>

**Molecular Weight:** 389.45

**Accurate Mass:** 389.195072

**Percentage Composition:** C 61.68%; H 6.99%; N 10.79%; O 20.54%

**Melting Point:** Mp 121-122°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>25</sup> +32.4 (c, 0.5 in CHCl<sub>3</sub>) (>98% de)

>>Derivative: *N*-Benzyloxycarbonyl, Me ester

**CAS Registry Number:** 28944-98-1

**Molecular Formula:** C<sub>23</sub>H<sub>25</sub>N<sub>3</sub>O<sub>5</sub>

**Molecular Weight:** 423.468

**Accurate Mass:** 423.179422

**Percentage Composition:** C 65.24%; H 5.95%; N 9.92%; O 18.89%

**Physical Description:** Cryst. (CHCl<sub>3</sub>/hexane)

**Melting Point:** Mp 120°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>25</sup> +44.7 (c, 0.5 in CHCl<sub>3</sub>)

>>Derivative: *N*-Benzyloxycarbonyl, benzyl ester

**Molecular Formula:** C<sub>29</sub>H<sub>29</sub>N<sub>3</sub>O<sub>5</sub>

**Molecular Weight:** 499.565

**Accurate Mass:** 499.210722

**Percentage Composition:** C 69.72%; H 5.85%; N 8.41%; O 16.01%

**Physical Description:** Cryst. (EtOAc/Et<sub>2</sub>O)

**Melting Point:** Mp 105°

#### References:

Abderhalden, E. *et al.*, *Hoppe Seyler's Z. Physiol. Chem.*, 1927, **171**, 93, (*synth*)

Gaudiano, G. *et al.*, *Gazz. Chim. Ital.*, 1957, **87**, 789, (*synth*)

Wilchek, M. *et al.*, *J.O.C.*, 1963, **28**, 1874, (*synth*)

Caballero, E. *et al.*, *Tetrahedron: Asymmetry*, 1998, **9**, 967-981, (*Me ester derivs, synth, pmr, cmr*)