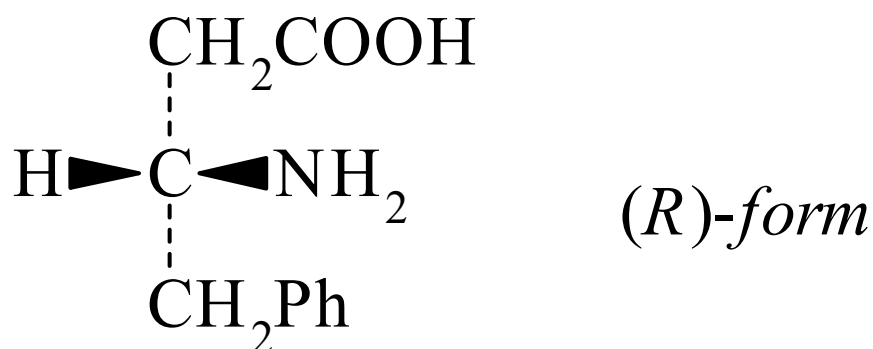




>>Entry Name: 3-Amino-4-phenylbutanoic acid, 8Cl

Synonym(s):  $\beta$ -Aminobenzenebutanoic acid, 9Cl.  $\beta$ -Homophenylalanine



**Molecular Formula:** C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub>

**Molecular Weight:** 179.218

**Accurate Mass:** 179.094629

**Percentage Composition:** C 67.02%; H 7.31%; N 7.82%; O 17.85%

>>Variant: (*R*)-form

**CAS Registry Number:** 131270-08-1

**Molecular Formula:** C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub>

**Molecular Weight:** 179.218

**Accurate Mass:** 179.094629

**Percentage Composition:** C 67.02%; H 7.31%; N 7.82%; O 17.85%

**Optical Rotation:**  $[\alpha]_D^{23}$  -8.5 (c, 0.2 in H<sub>2</sub>O)

>>Derivative: Me ester

**Molecular Formula:** C<sub>11</sub>H<sub>15</sub>NO<sub>2</sub>

**Molecular Weight:** 193.245

**Accurate Mass:** 193.110279

**Percentage Composition:** C 68.37%; H 7.82%; N 7.25%; O 16.56%

**Physical Description:** Cryst. (as hydrochloride)

**Melting Point:** Mp 133-134° (hydrochloride)

**Optical Rotation:**  $[\alpha]_D^{25}$  -9.2 (c, 1.5 in MeOH) (hydrochloride)

>>Variant: (*S*)-form

**CAS Registry Number:** 26250-87-3

**Molecular Formula:** C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub>

**Molecular Weight:** 179.218

**Accurate Mass:** 179.094629

**Percentage Composition:** C 67.02%; H 7.31%; N 7.82%; O 17.85%

**Physical Description:** Cryst. (EtOH aq.)

**Melting Point:** Mp 231-232° (225-226°)

**Optical Rotation:**  $[\alpha]_D$  +22.1 (c, 1.5 in H<sub>2</sub>O)

>>Derivative: *N*-9-Fluorenylmethoxycarbonyl

**CAS Registry Number:** 193954-28-8

**Molecular Formula:** C<sub>25</sub>H<sub>23</sub>NO<sub>4</sub>

**Molecular Weight:** 401.461

**Accurate Mass:** 401.162709

**Percentage Composition:** C 74.80%; H 5.77%; N 3.49%; O 15.94%

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

**Optical Rotation:**  $[\alpha]_D$  -19.3 (c, 1.23 in CHCl<sub>3</sub>)

>>Variant: ( $\pm$ )-form

**CAS Registry Number:** 131725-48-9

**Molecular Formula:** C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub>

**Molecular Weight:** 179.218

**Accurate Mass:** 179.094629

**Percentage Composition:** C 67.02%; H 7.31%; N 7.82%; O 17.85%

**Physical Description:** Cryst. (EtOH aq.)

**Melting Point:** Mp 226°