



**Boiling Point:** Bp<sub>0.75</sub> 115°  
**Optical Rotation:**  $[\alpha]_{\text{D}}^{25}$  -23.4 (c, 1.95 in MeOH)  
**Density:** d<sub>4</sub><sup>20</sup> 1.02  
**Refractive Index:** n<sub>D</sub><sup>20</sup> 1.5006

>>Derivative: Amide

**Synonym(s):** α-Aminobenzenepropanamide, 9Cl. Phenylalanine amide

**CAS Registry Number:** 5241-59-8  
**Molecular Formula:** C<sub>9</sub>H<sub>12</sub>N<sub>2</sub>O  
**Molecular Weight:** 164.207  
**Accurate Mass:** 164.094963  
**Percentage Composition:** C 65.83%; H 7.37%; N 17.06%; O 9.74%  
**Physical Description:** Cryst. (C<sub>6</sub>H<sub>6</sub>)  
**Melting Point:** Mp 91-93°  
**Optical Rotation:**  $[\alpha]_{\text{D}}^{24}$  -13.41 (MeOH)

>>Derivative: N-Formyl

**CAS Registry Number:** 59366-89-1  
**Molecular Formula:** C<sub>10</sub>H<sub>11</sub>NO<sub>3</sub>  
**Molecular Weight:** 193.202  
**Accurate Mass:** 193.073894  
**Percentage Composition:** C 62.17%; H 5.74%; N 7.25%; O 24.84%  
**Physical Description:** Plates (H<sub>2</sub>O)  
**Melting Point:** Mp 167°  
**Optical Rotation:**  $[\alpha]_{\text{D}}^{20}$  -75.2 (EtOH)

>>Derivative: N-Ac

**CAS Registry Number:** 10172-89-1  
**Molecular Formula:** C<sub>11</sub>H<sub>13</sub>NO<sub>3</sub>  
**Molecular Weight:** 207.229  
**Percentage Composition:** C 63.76%; H 6.32%; N 6.76%; O 23.16%  
**Melting Point:** Mp 170-171°  
**Optical Rotation:**  $[\alpha]_{\text{D}}$  -49.3  
**Sigma:** A3876

>>Derivative: N-Ac, Me ester

**CAS Registry Number:** 21156-62-7  
**Molecular Formula:** C<sub>12</sub>H<sub>15</sub>NO<sub>3</sub>  
**Molecular Weight:** 221.255  
**Accurate Mass:** 221.105194  
**Percentage Composition:** C 65.14%; H 6.83%; N 6.33%; O 21.69%  
**Physical Description:** Prisms (Et<sub>2</sub>O)  
**Melting Point:** Mp 90-91°  
**Optical Rotation:**  $[\alpha]_{\text{D}}^{25}$  -19 (c, 2 in MeOH)

>>Derivative: N-Ac, Et ester

**CAS Registry Number:** 20918-84-7  
**Molecular Formula:** C<sub>13</sub>H<sub>17</sub>NO<sub>3</sub>  
**Molecular Weight:** 235.282  
**Accurate Mass:** 235.120844  
**Percentage Composition:** C 66.36%; H 7.28%; N 5.95%; O 20.40%  
**Physical Description:** Cryst.  
**Melting Point:** Mp 93.5-94.5°  
**Optical Rotation:**  $[\alpha]_{\text{D}}^{25}$  -61.8 (c, 1 in CHCl<sub>3</sub>) (72% ee)

>>Derivative: N-Benzoyl

**CAS Registry Number:** 37002-52-1  
**Molecular Formula:** C<sub>16</sub>H<sub>15</sub>NO<sub>3</sub>  
**Molecular Weight:** 269.299  
**Percentage Composition:** C 71.36%; H 5.61%; N 5.20%; O 17.82%  
**Physical Description:** Needles (H<sub>2</sub>O)  
**Melting Point:** Mp 154-155° (146-148°)  
**Optical Rotation:**  $[\alpha]$