



Physical Description: Oil
Optical Rotation: $[\alpha]_{\text{D}}^{18} -15.5$ (neat)

>>**Variant:** (S)-form

CAS Registry Number: 40856-44-8
Molecular Formula: $\text{C}_9\text{H}_{11}\text{NO}_2$
Molecular Weight: 165.191
Accurate Mass: 165.078979
Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%
Physical Description: Cryst. (H_2O)
Melting Point: Mp 234-235°
Optical Rotation: $[\alpha]_{\text{D}}^{25} -7.5$ (H_2O)

>>**Derivative:** N-Me
Synonym(s): 3-(Methylamino)-3-phenylpropanoic acid

Molecular Formula: $\text{C}_{10}\text{H}_{13}\text{NO}_2$
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. (MeOH/Et₂O)
Melting Point: Mp 162°
Optical Rotation: $[\alpha]_{\text{D}} -47$ (c, 1.7 in MeOH)

>>**Derivative:** N-Ph
Synonym(s): 3-Anilino-3-phenylpropanoic acid

Molecular Formula: $\text{C}_{15}\text{H}_{15}\text{NO}_2$
Molecular Weight: 241.289
Accurate Mass: 241.110279
Percentage Composition: C 74.67%; H 6.27%; N 5.80%; O 13.26%
Physical Description: Solid
Melting Point: Mp 125-126°

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

Molecular Formula: $\text{C}_{16}\text{H}_{17}\text{NO}_2$
Molecular Weight: 255.316
Accurate Mass: 255.125929
Percentage Composition: C 75.27%; H 6.71%; N 5.49%; O 12.53%
Physical Description: Solid
Melting Point: Mp 113-114°

>>**Variant:** (±)-form

CAS Registry Number: 3646-50-2
Molecular Formula: $\text{C}_9\text{H}_{11}\text{NO}_2$
Molecular Weight: 165.191
Accurate Mass: 165.078979
Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%
Physical Description: Cryst. (H_2O)
Melting Point: Mp 231°
Solubility: Sol. hot H_2O

>>**Derivative:** Hydrochloride

Physical Description: Prisms (EtOH)
Melting Point: Mp 218°

>>**Derivative:** Amide

Molecular Formula: $\text{C}_9\text{H}_{12}\text{N}_2\text{O}$
Molecular Weight: 164.207
Accurate Mass: 164.094963
Percentage Composition: C 65.83%; H 7.37%; N 17.06%; O 9.74%
Melting Point: Mp 196-196.5 dec.°