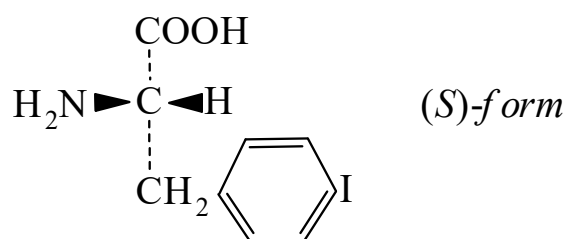




>>Entry Name: 2-Amino-3-(4-iodophenyl)propanoic acid

Synonym(s): 4-Iodophenylalanine, 9Cl. NGW05



CAS Registry Number: 1991-81-7

Related CAS Registry Numbers(s): 82611-58-3 98833-69-3 103882-09-3 113850-77-4

Molecular Formula: C<sub>9</sub>H<sub>10</sub>INO<sub>2</sub>

Molecular Weight: 291.088

Accurate Mass: 290.975627

Percentage Composition: C 37.14%; H 3.46%; I 43.60%; N 4.81%; O 10.99%

>>Variant: (R)-form

Synonym(s): D-form

CAS Registry Number: 62561-75-5

Molecular Formula: C<sub>9</sub>H<sub>10</sub>INO<sub>2</sub>

Molecular Weight: 291.088

Accurate Mass: 290.975627

Percentage Composition: C 37.14%; H 3.46%; I 43.60%; N 4.81%; O 10.99%

Melting Point: Mp 251° (dec.)

Optical Rotation:  $[\alpha]_D^{25} -22$  (c, 1 in 1M HCl/EtOH (1:1))

Other Data: The opt. rotation cited is prob. erroneous comparing lit. values for the (S)-form and for the (R)-forms of the fluoro, chloro and bromo analogues

>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 24250-85-9

Molecular Formula: C<sub>9</sub>H<sub>10</sub>INO<sub>2</sub>

Molecular Weight: 291.088

Accurate Mass: 290.975627

Percentage Composition: C 37.14%; H 3.46%; I 43.60%; N 4.81%; O 10.99%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 261-262° (232-234°)

Optical Rotation:  $[\alpha]_D^{22} -9.1$  (c, 0.65 in 80% AcOH)

Sigma: I8757

>>Derivative: Me ester

CAS Registry Number: 158686-46-5

Molecular Formula: C<sub>10</sub>H<sub>12</sub>INO<sub>2</sub>

Molecular Weight: 305.115

Accurate Mass: 304.991277

Percentage Composition: C 39.37%; H 3.96%; I 41.59%; N 4.59%; O 10.49%

Physical Description: Cryst. (MeOH/Et<sub>2</sub>O) (as hydrochloride)

Melting Point: Mp 199.5-200.5° (hydrochloride)

Other Data: CAS no. refers to hydrochloride

>>Derivative: tert-Butyl ester

CAS Registry Number: 115819-99-3

Molecular Formula: C<sub>13</sub>H<sub>18</sub>INO<sub>2</sub>

Molecular Weight: 347.195

Accurate Mass: 347.038227

Percentage Composition: C 44.97%; H 5.23%; I 36.55%; N 4.03%; O 9.22%

Physical Description: Flakes (H<sub>2</sub>O) (as hydrochloride)

Melting Point: Mp 233° (dec.) (hydrochloride)

Other Data: CAS no. refers to hydrochloride