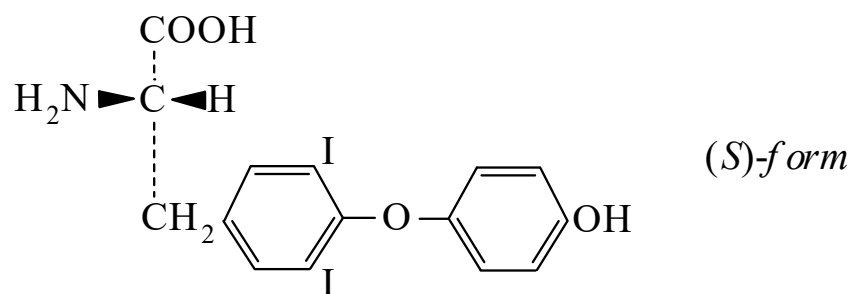




>>Entry Name: 3,5-Diiodothyronine

Synonym(s): *O*-(4-Hydroxyphenyl)-3,5-diiodotyrosine, 9CI. β -[4-(*p*-Hydroxyphenoxy)-3,5-diiodophenyl]alanine



CAS Registry Number: 534-51-0

Related CAS Registry Numbers(s): 5563-89-3

Molecular Formula: $C_{15}H_{13}I_2NO_4$

Molecular Weight: 525.081

Accurate Mass: 524.893405

Percentage Composition: C 34.31%; H 2.50%; I 48.34%; N 2.67%; O 12.19%

Other: PB D31750

>>Variant: (*R*)-form

Synonym(s): D-form

Molecular Formula: $C_{15}H_{13}I_2NO_4$

Molecular Weight: 525.081

Accurate Mass: 524.893405

Percentage Composition: C 34.31%; H 2.50%; I 48.34%; N 2.67%; O 12.19%

Melting Point: Mp 265 dec.°

Optical Rotation: $[\alpha]_D^{20} -27.1$ (c, 1 in 0.35*M* EtOH/HCl)

>>Derivative: *N*-Ac

Molecular Formula: $C_{17}H_{15}I_2NO_5$

Molecular Weight: 567.118

Accurate Mass: 566.90397

Percentage Composition: C 36.00%; H 2.67%; I 44.75%; N 2.47%; O 14.11%

Melting Point: Mp 143-145°

Optical Rotation: $[\alpha]_D^{19} -30.5$ (c, 6 in dioxan)

>>Derivative: Et ester

Molecular Formula: $C_{17}H_{17}I_2NO_4$

Molecular Weight: 553.135

Accurate Mass: 552.924705

Percentage Composition: C 36.91%; H 3.10%; I 45.89%; N 2.53%; O 11.57%

Melting Point: Mp 132-136°

Optical Rotation: $[\alpha]_D^{19} -43.4$ (c, 0.99 in dioxan)

>>Variant: (*S*)-form

Synonym(s): L-form

CAS Registry Number: 1041-01-6

Type of Compound Code(s): AH0100 VV0100

Molecular Formula: $C_{15}H_{13}I_2NO_4$

Molecular Weight: 525.081

Accurate Mass: 524.893405

Percentage Composition: C 34.31%; H 2.50%; I 48.34%; N 2.67%; O 12.19%

Biological Source: Occurs in proteins of marine algae

Melting Point: Mp 255 dec.°

Fluka: 38100

Sigma: D0629