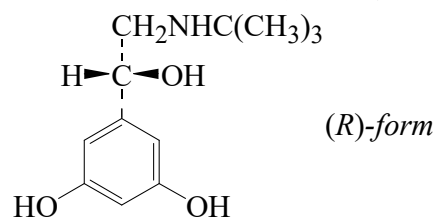




>>Entry Name: Terbutaline, BAN, INN

Synonym(s): 5-[2-[(1,1-Dimethylethyl)amino]-1-hydroxyethyl]-1,3-benzenediol, 9CI. α -[(*tert*-Butylamino)methyl]-3,5-dihydroxybenzyl alcohol, 8CI



CAS Registry Number: 23031-25-6

Related CAS Registry Numbers(s): 57576-17-7 59969-41-4 61435-51-6

Molecular Formula: $\text{C}_{12}\text{H}_{19}\text{NO}_3$

Molecular Weight: 225.287

Accurate Mass: 225.136494

Percentage Composition: C 63.98%; H 8.50%; N 6.22%; O 21.31%

Biological Use/Importance: β -Adrenoceptor agonist. Sympathomimetic. Used to prevent pulmonary oedema caused by phosgene

Development Status: Approved 1974

Calculated Log P Data: Log P 0.48 (calc)

Hazard & Toxicity: Human reprod. and other adverse effects when used therapeutically

>>Variant: (*R*)-form

CAS Registry Number: 37394-31-3

Molecular Formula: $\text{C}_{12}\text{H}_{19}\text{NO}_3$

Molecular Weight: 225.287

Accurate Mass: 225.136494

Percentage Composition: C 63.98%; H 8.50%; N 6.22%; O 21.31%

Other Data: More active than the (+)-form

>>Derivative: Hydrobromide

CAS Registry Number: 39986-53-3

Physical Description: Cryst. (EtOH/Et₂O)

Optical Rotation: $[\alpha]_{\text{D}}^{20} -34.6$ (c, 1 in MeOH)

>>Derivative: Hydrochloride

Melting Point: Mp 215° (dec.)

Optical Rotation: $[\alpha]_{\text{D}}^{20} -32.5$ (c, 0.76 in MeOH) (>98% ee)

>>Variant: (*S*)-form

CAS Registry Number: 90877-48-8

Molecular Formula: $\text{C}_{12}\text{H}_{19}\text{NO}_3$

Molecular Weight: 225.287

Accurate Mass: 225.136494

Percentage Composition: C 63.98%; H 8.50%; N 6.22%; O 21.31%

>>Derivative: Hydrobromide

CAS Registry Number: 39986-54-4

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 241-243°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +34.2$ (c, 1.0 in MeOH)

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

CAS Registry Number: 46719-29-3

Molecular Formula: $\text{C}_{12}\text{H}_{19}\text{NO}_3$

Molecular Weight: 225.287

Accurate Mass: 225.136494

Percentage Composition: C 63.98%; H 8.50%; N 6.22%; O 21.31%

Melting Point: Mp 119-122°