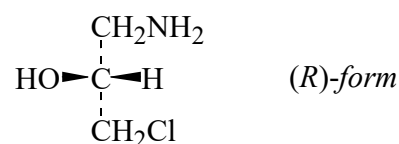




>>Entry Name: 1-Amino-3-chloro-2-propanol, 9Cl



CAS Registry Number: 3920-12-5

Related CAS Registry Numbers(s): 54868-31-4

Molecular Formula: C<sub>3</sub>H<sub>8</sub>ClNO

Molecular Weight: 109.555

Accurate Mass: 109.029441

Percentage Composition: C 32.89%; H 7.36%; Cl 32.36%; N 12.79%; O 14.60%

>>Variant: (R)-form

Molecular Formula: C<sub>3</sub>H<sub>8</sub>ClNO

Molecular Weight: 109.555

Accurate Mass: 109.029441

Percentage Composition: C 32.89%; H 7.36%; Cl 32.36%; N 12.79%; O 14.60%

>>Derivative: *N,N,N*-Tri-Me

Synonym(s): 3-Chloro-2-hydroxy-*N,N,N*-trimethyl-1-propanaminium, 9Cl. (3-Chloro-2-hydroxypropyl)trimethylammonium(1+), 8Cl

CAS Registry Number: 117604-42-9

Molecular Formula: C<sub>6</sub>H<sub>15</sub>ClNO<sup>(+)</sup>

Molecular Weight: 152.643

Accurate Mass: 152.084216

Percentage Composition: C 47.21%; H 9.90%; Cl 23.23%; N 9.18%; O 10.48%

Melting Point: Mp 217° (dec.) (as chloride)

Optical Rotation:  $[\alpha]_{\text{D}}^{25} +29$  (c, 1 in H<sub>2</sub>O) (chloride)

Other Data: CAS no. refers to chloride

Aldrich: 32916-9

>>Variant: (S)-form

CAS Registry Number: 53494-57-8

Molecular Formula: C<sub>3</sub>H<sub>8</sub>ClNO

Molecular Weight: 109.555

Accurate Mass: 109.029441

Percentage Composition: C 32.89%; H 7.36%; Cl 32.36%; N 12.79%; O 14.60%

>>Derivative: *N,N,N*-Tri-Me, chloride

CAS Registry Number: 101396-91-2

Molecular Formula: C<sub>6</sub>H<sub>15</sub>Cl<sub>2</sub>NO

Molecular Weight: 188.096

Accurate Mass: 187.053068

Percentage Composition: C 38.31%; H 8.04%; Cl 37.70%; N 7.45%; O 8.51%

Use/Importance: Intermed. in synth. of [BDS82-P](#)

Physical Description: Cryst. (EtOH)

Melting Point: Mp 212-214°

Optical Rotation:  $[\alpha]_{\text{D}}^{25} -30.2$  (c, 1 in H<sub>2</sub>O)

Aldrich: 32917-7

>>Derivative: *N,N,N*-Tri-Me, tartrate salt

Physical Description: Cryst. (MeOH/Me<sub>2</sub>CO) (as hydrogen tartrate)

Melting Point: Mp 152-153° (hydrogen tartrate)

Optical Rotation:  $[\alpha]_{\text{D}}^{25} -10.7$  (c, 1 in H<sub>2</sub>O) (hydrogen tartrate)

>>Variant: (±)-form

CAS Registry Number: 59348-49-1

Molecular Formula: C<sub>3</sub>H<sub>8</sub>ClNO

Molecular Weight: 109.555

Accurate Mass: 109.029441

Percentage Composition: C 32.89%; H 7.36%; Cl 32.36%; N 12.79%; O 14.60%