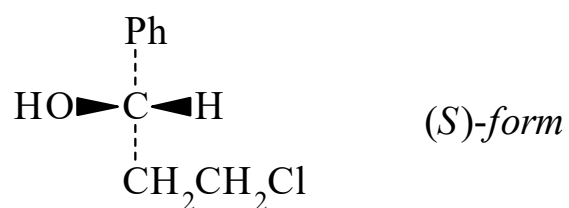




>>Entry Name: 3-Chloro-1-phenyl-1-propanol

Synonym(s): α -(2-Chloroethyl)benzenemethanol, 9Cl. 2-Chloroethylphenylmethanol



CAS Registry Number: 18776-12-0

Related CAS Registry Numbers(s): 100306-33-0

Molecular Formula: C₉H₁₁ClO

Molecular Weight: 170.638

Accurate Mass: 170.049842

Percentage Composition: C 63.35%; H 6.50%; Cl 20.78%; O 9.38%

>>Variant: (S)-form

CAS Registry Number: 100306-34-1

Molecular Formula: C₉H₁₁ClO

Molecular Weight: 170.638

Accurate Mass: 170.049842

Percentage Composition: C 63.35%; H 6.50%; Cl 20.78%; O 9.38%

Optical Rotation: $[\alpha]_{\text{D}}^{19} -24.7$ (c, 1 in CHCl₃)

Aldrich: 32461-2

>>Variant: (±)-form

Molecular Formula: C₉H₁₁ClO

Molecular Weight: 170.638

Accurate Mass: 170.049842

Percentage Composition: C 63.35%; H 6.50%; Cl 20.78%; O 9.38%

Physical Description: Liq.

Boiling Point: Bp₈ 130-132°. Bp_{0.1} 90-93°

>>Derivative: 4-Nitrobenzoyl

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 62-63°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 332A, (*nmr*)

Case, F.H., *J.A.C.S.*, 1933, **55**, 2927, (*synth*)

Soai, K. *et al.*, *Chem. Comm.*, 1986, 1018, (*synth, abs config*)

Robertson, D.W. *et al.*, *J. Med. Chem.*, 1988, **31**, 1412, (*synth*)

Wirth, D.D. *et al.*, *Org. Process Res. Dev.*, 2000, **4**, 513-519, (*synth, pmr, cmr*)