



>>Entry Name: **3-Chloro-1-phenylpropene**

Synonym(s): (3-Chloro-1-propenyl)benzene, 9Cl. Cinnamyl chloride. γ -Chloropropenylbenzene

CAS Registry Number: 2687-12-9

PhCH=CHCH₂Cl

Molecular Formula: C₉H₉Cl

Molecular Weight: 152.623

Accurate Mass: 152.039277

Percentage Composition: C 70.83%; H 5.94%; Cl 23.23%

Hazard & Toxicity: Fl. p. >66°

Aldrich: 18718-6

>>Variant: (E)-form

CAS Registry Number: 21087-29-6

Molecular Formula: C₉H₉Cl

Molecular Weight: 152.623

Accurate Mass: 152.039277

Percentage Composition: C 70.83%; H 5.94%; Cl 23.23%

Physical Description: Pale yellow oil or needles

Melting Point: Mp 8-9°

Boiling Point: Bp₂₂ 125-126°. Bp_{0.7} 55-56°

>>Variant: (Z)-form

CAS Registry Number: 39199-93-4

Molecular Formula: C₉H₉Cl

Molecular Weight: 152.623

Accurate Mass: 152.039277

Percentage Composition: C 70.83%; H 5.94%; Cl 23.23%

Physical Description: Liq.

Boiling Point: Bp₆ 80-90°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 136B, (*nmr*)

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Lehmkuhl, H. *et al.*, *Annalen*, 1978, 1449

Abbott, F.S. *et al.*, *Can. J. Chem.*, 1978, **56**, 71, (*config*)

Hutchins, R.O. *et al.*, *J.O.C.*, 1978, **43**, 2259

Dehmlow, E.V. *et al.*, *Annalen*, 1980, 1

Davis, F.A. *et al.*, *J.O.C.*, 1992, **57**, 2599, (*synth, ir, pmr*)