



>>Entry Name: 3-(2,6-Dichlorophenyl)-2-propenoic acid, 9Cl

Synonym(s): 2,6-Dichlorocinnamic acid, 8Cl

CAS Registry Number: 5345-89-1

Molecular Formula: C₉H₆Cl₂O₂

Molecular Weight: 217.051

Accurate Mass: 215.974484

Percentage Composition: C 49.80%; H 2.79%; Cl 32.67%; O 14.74%

>>Variant: (*E*)-form

CAS Registry Number: 20595-49-7

Molecular Formula: C₉H₆Cl₂O₂

Molecular Weight: 217.051

Accurate Mass: 215.974484

Percentage Composition: C 49.80%; H 2.79%; Cl 32.67%; O 14.74%

Melting Point: Mp 195°

>>Variant: (*Z*)-form

CAS Registry Number: 20595-50-0

Molecular Formula: C₉H₆Cl₂O₂

Molecular Weight: 217.051

Accurate Mass: 215.974484

Percentage Composition: C 49.80%; H 2.79%; Cl 32.67%; O 14.74%

Melting Point: Mp 164-165°

>>Derivative: Nitrile

CAS Registry Number: 58177-60-9

Molecular Formula: C₉H₅Cl₂N

Molecular Weight: 198.051

Accurate Mass: 196.979903

Percentage Composition: C 54.58%; H 2.54%; Cl 35.80%; N 7.07%

Melting Point: Mp 25-26°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1054B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 182C, (*ir*)

Ugochukwu, E.N. *et al.*, *Ann. Appl. Biol.*, 1968, **61**, 121, (*synth*)

Fairhurst, J. *et al.*, *Tet. Lett.*, 1975, 3843, (*synth*)