



>>Entry Name: 3-(2,4-Dichlorophenyl)-2-propenoic acid, 9Cl

Synonym(s): 2,4-Dichlorocinnamic acid, 8Cl

CAS Registry Number: 1201-99-6

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%

Sigma: D0396

>>Variant: (E)-form

CAS Registry Number: 20595-45-3

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 239-240.5°

Aldrich: 14462-2

>>Derivative: Et ester

CAS Registry Number: 24393-62-2

Molecular Formula: C₁₁H₁₀Cl₂O₂

Molecular Weight: 245.104

Accurate Mass: 244.005784

Percentage Composition: C 53.90%; H 4.11%; Cl 28.93%; O 13.06%

Melting Point: Mp 53.5°

Boiling Point: Bp₅ 162°

>>Derivative: Chloride

CAS Registry Number: 39175-64-9

Molecular Formula: C₉H₅Cl₃O

Molecular Weight: 235.496

Accurate Mass: 233.940596

Percentage Composition: C 45.90%; H 2.14%; Cl 45.16%; O 6.79%

Melting Point: Mp 81-82°

>>Variant: (Z)-form

CAS Registry Number: 20595-46-4

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 132-133°

References:

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

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

Walling, C. *et al.*, *J.A.C.S.*, 1947, **69**, 852, (*synth*)

Lindenfors, S., *Ark. Kemi*, 1957, **10**, 561, (*synth, ir*)

Org. Synth., Coll. Vol., 4, 1963, 731

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

Phillips, W.M. *et al.*, *Can. J. Chem.*, 1969, **47**, 3137, (*nmr*)