



>>Entry Name: 3-(3-Chlorophenyl)propanoic acid

Synonym(s): 3-Chlorobenzenepropanoic acid, 9Cl. *m*-Chlorohydrocinnamic acid, 8Cl. 3-*m*-Chlorophenylpropionic acid

CAS Registry Number: 21640-48-2

Structure by analogy with 3-(2-Chlorophenyl)propanoic acid, [DXD04-C](#)

Molecular Formula: C<sub>9</sub>H<sub>9</sub>ClO<sub>2</sub>

Molecular Weight: 184.622

Accurate Mass: 184.029107

Percentage Composition: C 58.55%; H 4.91%; Cl 19.20%; O 17.33%

Physical Description: Leaflets (petrol) or prisms

Melting Point: Mp 77-78° (73-74°)

pKa Value: pK<sub>a</sub> 4.59

>>Derivative: Et ester

CAS Registry Number: 7116-35-0

Molecular Formula: C<sub>11</sub>H<sub>13</sub>ClO<sub>2</sub>

Molecular Weight: 212.675

Accurate Mass: 212.060407

Percentage Composition: C 62.12%; H 6.16%; Cl 16.67%; O 15.05%

Physical Description: Liq.

Boiling Point: Bp<sub>5</sub> 124-130°

>>Derivative: Chloride

CAS Registry Number: 40478-50-0

Molecular Formula: C<sub>9</sub>H<sub>8</sub>Cl<sub>2</sub>O

Molecular Weight: 203.067

Accurate Mass: 201.995219

Percentage Composition: C 53.23%; H 3.97%; Cl 34.92%; O 7.88%

Physical Description: Liq.

Boiling Point: Bp<sub>39</sub> 161°

>>Derivative: Anilide

Molecular Formula: C<sub>15</sub>H<sub>14</sub>ClNO

Molecular Weight: 259.734

Accurate Mass: 259.076391

Percentage Composition: C 69.37%; H 5.43%; Cl 13.65%; N 5.39%; O 6.16%

Melting Point: Mp 86-87°

References:

Kenner, J. *et al.*, *J.C.S.*, 1921, **119**, 1460, (*synth*)

Dippy, J.F. *et al.*, *J.C.S.*, 1938, 357, (*synth*)

Fuchs, R. *et al.*, *J.O.C.*, 1962, **27**, 733, (*synth*)

Kadentsev, V.I. *et al.*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1972, 2440; *CA*, **78**, 96726, (*ms*)