



>>Entry Name: 3-Formylbenzoic acid, 9Cl

Synonym(s): Isophthalaldehydic acid, 8Cl. Benzaldehyde-*m*-carboxylic acid

CAS Registry Number: 619-21-6

Structure by analogy with 2-Formylbenzoic acid, [DTP57-A](#)

Molecular Formula: C₈H₆O₃

Molecular Weight: 150.134

Accurate Mass: 150.031695

Percentage Composition: C 64.00%; H 4.03%; O 31.97%

Physical Description: Needles (H₂O)

Melting Point: Mp 175°

pKa Value: pK_{a1} 3.84 (25°)

Aldrich: 23279-3

Fluka: 21869

>>Derivative: Oxime

Molecular Formula: C₈H₇NO₃

Molecular Weight: 165.148

Accurate Mass: 165.042594

Percentage Composition: C 58.18%; H 4.27%; N 8.48%; O 29.06%

Melting Point: Mp 188°

>>Derivative: Phenylhydrazone

Melting Point: Mp 164°

>>Derivative: Me ester

CAS Registry Number: 52178-50-4

Molecular Formula: C₉H₈O₃

Molecular Weight: 164.16

Accurate Mass: 164.047345

Percentage Composition: C 65.85%; H 4.91%; O 29.24%

Melting Point: Mp 53°

>>Derivative: Et ester

CAS Registry Number: 33745-47-0

Molecular Formula: C₁₀H₁₀O₃

Molecular Weight: 178.187

Accurate Mass: 178.062995

Percentage Composition: C 67.41%; H 5.66%; O 26.94%

Boiling Point: Bp 278°

Density: d¹⁸ 1.093

>>Derivative: Chloride

CAS Registry Number: 75650-38-3

Molecular Formula: C₈H₅ClO₂

Molecular Weight: 168.579

Accurate Mass: 167.997807

Percentage Composition: C 57.00%; H 2.99%; Cl 21.03%; O 18.98%

Boiling Point: Bp₂₀ 130°

>>Derivative: Amide

Molecular Formula: C₈H₇NO₂

Molecular Weight: 149.149

Accurate Mass: 149.047679

Percentage Composition: C 64.42%; H 4.73%; N 9.39%; O 21.45%

Physical Description: Prisms

Melting Point: Mp 190 dec.°

>>Derivative: Nitrile