



>>Entry Name: 4-Formylbenzoic acid, 9Cl

Synonym(s): Terephthalaldehydic acid, 8Cl. Benzaldehyde-*p*-carboxylic acid. *p*-Carboxybenzaldehyde. *p*-CBA

CAS Registry Number: 619-66-9

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

Molecular Formula: C<sub>8</sub>H<sub>6</sub>O<sub>3</sub>

Molecular Weight: 150.134

Accurate Mass: 150.031695

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

Use/Importance: V. reactive aromatic aldehyde used extensively in synthesis

Physical Description: Needles (H<sub>2</sub>O)

Melting Point: Mp 256°

pKa Value: pK<sub>a1</sub> 3.77 (25°)

Aldrich: 12491-5

Fluka: 21870

Sigma: C1904

>>Derivative: Oxime

CAS Registry Number: 3477-93-8

Molecular Formula: C<sub>8</sub>H<sub>7</sub>NO<sub>3</sub>

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 208-210°

>>Derivative: Phenylhydrazone

CAS Registry Number: 61471-39-4

Melting Point: Mp 226°

>>Derivative: Me ester

CAS Registry Number: 1571-08-0

Molecular Formula: C<sub>9</sub>H<sub>8</sub>O<sub>3</sub>

Molecular Weight: 164.16

Accurate Mass: 164.047345

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

Physical Description: Needles (H<sub>2</sub>O or petrol)

Melting Point: Mp 63°

Boiling Point: Bp 265°

Aldrich: 24474-0

Fluka: 47717

>>Derivative: Chloride

CAS Registry Number: 16173-52-7

Molecular Formula: C<sub>8</sub>H<sub>5</sub>ClO<sub>2</sub>

Molecular Weight: 168.579

Accurate Mass: 167.997807

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

Melting Point: Mp 48°

Boiling Point: Bp 258°

>>Derivative: Nitrile

see 4-Cyanobenzaldehyde, [DXH57-O](#)

References: