



>>Entry Name: 1,4-Benzenedicarboxaldehyde, 9CI
Synonym(s): Terephthalaldehyde, 8CI. 1,4-Diformylbenzene

CAS Registry Number: 623-27-8

Molecular Formula: C₈H₆O₂
Molecular Weight: 134.134
Accurate Mass: 134.03678
Percentage Composition: C 71.64%; H 4.51%; O 23.86%
Physical Description: Cryst. (H₂O)
Melting Point: Mp 116°
Boiling Point: Bp 245-248°
Other Data: Sublimes

Aldrich: T220-7
Fluka: 86410

>>Derivative: Dioxime

CAS Registry Number: 18705-39-0
Molecular Formula: C₈H₈N₂O₂
Molecular Weight: 164.163
Accurate Mass: 164.058578
Percentage Composition: C 58.53%; H 4.91%; N 17.06%; O 19.49%
Physical Description: Cryst.
Melting Point: Mp 200°

>>Derivative: Monophenylhydrazone

Physical Description: Orange-yellow cryst. (Et₂O)
Melting Point: Mp 152-154°

>>Derivative: Bisphenylhydrazone

CAS Registry Number: 7265-27-2
Physical Description: Yellow cryst. (AcOH)
Melting Point: Mp 278°

>>Derivative: Bis(4-nitrophenyl)hydrazone

Physical Description: Cryst. (PhNO₂)
Melting Point: Mp 281° (sinters at 272°)

>>Derivative: Mono(di-Et acetal)
Synonym(s): 4-(Diethoxymethyl)benzaldehyde

CAS Registry Number: 81172-89-6
Molecular Formula: C₁₂H₁₆O₃
Molecular Weight: 208.257
Accurate Mass: 208.109945
Percentage Composition: C 69.21%; H 7.74%; O 23.05%
Physical Description: Liq.
Density: d 1.05
Refractive Index: n_D²⁰ 1.5060

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 945B, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 113A, (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1293A, (*ir*)
Adams, R. *et al.*, *J.A.C.S.*, 1923, **45**, 521, (*synth*)
Org. Synth., Coll. Vol., 3, 1955, 788, (*synth*)
Costa, L. *et al.*, *Heterocycl. Chem.*, 1974, **11**, 943, (*synth*)
Schoenberg, A. *et al.*, *J.A.C.S.*, 1974, **96**, 7761, (*synth*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, TAN500