



>>Entry Name: 9-Anthracenecarboxaldehyde, 9CI

Synonym(s): 9-Anthraldehyde, 8CI

CAS Registry Number: 642-31-9

Molecular Formula: C₁₅H₁₀O

Molecular Weight: 206.243

Accurate Mass: 206.073165

Percentage Composition: C 87.36%; H 4.89%; O 7.76%

Physical Description: Orange needles (AcOH)

Melting Point: Mp 104-105°

pKa Value: pK_a -4.81 (H₂SO₄ aq.)

Other Data: Dec. by light

Aldrich: 27868-8

Fluka: 10603

Rare Chemicals Library: S5899-9

Sigma: A8912

>>Derivative: (E)-Oxime

CAS Registry Number: 1942-19-4

Molecular Formula: C₁₅H₁₁NO

Molecular Weight: 221.258

Accurate Mass: 221.084064

Percentage Composition: C 81.43%; H 5.01%; N 6.33%; O 7.23%

Physical Description: Cryst. (EtOH or C₆H₆)

Melting Point: Mp 260-262°

>>Derivative: (Z)-Oxime

CAS Registry Number: 2497-53-2

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 165-166°

>>Derivative: Hydrazone

CAS Registry Number: 7512-18-7

Molecular Formula: C₁₅H₁₂N₂

Molecular Weight: 220.273

Accurate Mass: 220.100048

Percentage Composition: C 81.79%; H 5.49%; N 12.72%

Physical Description: Orange cryst. (EtOH)

Melting Point: Mp 124-126°

>>Derivative: Phenylhydrazone

CAS Registry Number: 10208-19-2

Physical Description: Orange needles (EtOH)

Melting Point: Mp 207°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 978C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1313D, (*ir*)

Hinkel, L.E. *et al.*, *J.C.S.*, 1936, 344, (*synth, derivs*)

Campaigne, E. *et al.*, *J.A.C.S.*, 1953, **75**, 989, (*synth*)

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Trotter, J., *Acta Cryst. C*, 1959, **12**, 922, (*cryst struct*)