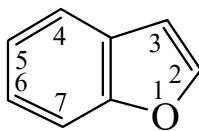




>>Entry Name: Benzofuran, 9CI

Synonym(s): Coumarone. Benzo[b]furan. Benzofurfuran. 1-Oxaindene. 1-Oxindene



CAS Registry Number: 271-89-6

Molecular Formula: C₈H₆O

Molecular Weight: 118.135

Accurate Mass: 118.041865

Percentage Composition: C 81.34%; H 5.12%; O 13.54%

Biological Source: Constit. of *Coix lachryma-jobi*, *Gentiana lutea*, *Michelia alba* and *Trilisa odoratissima*

Physical Description: Oil

Boiling Point: Bp₇₃₅ 166.5-168°. Bp₈₀ 97.5-99°

Density: d₄¹⁵ 1.078

Other Data: Steam-volatile. Stable to alkalis, polymerised by H₂SO₄

Hazard & Toxicity: LD₅₀ (mus, ipr) 500 mg/kg

Aldrich: B800-2

Fluka: 28165

Sigma: B0139

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 683B, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 168C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1505A, (*ir*)

Badger, G.M. *et al.*, *J.C.S.*, 1956, 3438, (*uv*)

Black, P.J. *et al.*, *Aust. J. Chem.*, 1965, **18**, 353, (*pmr*)

Org. Synth., 1966, **46**, 28, (*synth, uv*)

Appleton, R.A. *et al.*, *Phytochemistry*, 1971, **10**, 447-449, (*isol*)

Platzer, N. *et al.*, *Bull. Soc. Chim. Fr.*, 1974, 905, (*cmr*)

Cagniant, P. *et al.*, *Adv. Heterocycl. Chem.*, 1975, **18**, 337, (*rev*)

Kuster, T. *et al.*, *Helv. Chim. Acta*, 1978, **61**, 1017, (*ms*)

Audit, M. *et al.*, *Org. Magn. Reson.*, 1983, **21**, 698, (*pmr*)

Fraser, R.R. *et al.*, *Can. J. Chem.*, 1985, **63**, 3505, (*cmr*)

Kreher, R.P. *et al.*, *Chem. Ber.*, 1991, **124**, 645, (*bibl*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, BCK250