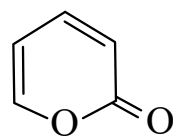




>>Entry Name: **2*H*-Pyran-2-one**, 9CI, 8CI

Synonym(s): Coumalin. α -Pyrone. 2-Pyrone



CAS Registry Number: 504-31-4

Molecular Formula: C₅H₄O₂

Molecular Weight: 96.085

Accurate Mass: 96.02113

Percentage Composition: C 62.50%; H 4.20%; O 33.30%

Use/Importance: Diels-Alder diene

Physical Description: Oil

Melting Point: Mp 5°

Boiling Point: Bp 206-209° sl. dec.. Bp₂₆ 110°

Solubility: Misc. H₂O

Density: d₄²⁰ 1.2

Refractive Index: n_D²⁰ 1.5298

Aldrich: 46315-9

Fluka: 83193

References:

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 756D, (*ir*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 970

Evnin, A.B. *et al.*, *J.A.C.S.*, 1967, **89**, 952, (*synth*, *ir*, *pmr*)

Pirkle, W.H. *et al.*, *J. Het. Chem.*, 1969, **6**, 1, (*pmr*)

Pirkle, W.H. *et al.*, *J.O.C.*, 1974, **39**, 1935, (*cmr*)

Nakagawa, M. *et al.*, *Synthesis*, 1974, 510, (*synth*)

Izumi, T. *et al.*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 1673, (*synth*)

Org. Synth., 1977, **56**, 49, (*synth*)

Holmes, J.H. *et al.*, *J.A.C.S.*, 1979, **101**, 4973, (*ms*)

Imagawa, T. *et al.*, *Org. Magn. Reson.*, 1980, **13**, 244, (*cmr*, *pmr*)

Nakazumi, H. *et al.*, *Phosphorus Sulfur Relat. Elem.*, 1983, **16**, 59, (*uv*)

Blake, A.J. *et al.*, *Acta Cryst. C*, 1994, **50**, 1938, (*cryst struct*)

Kotretsou, S.I. *et al.*, *Org. Prep. Proced. Int.*, 2000, **32**, 161-167, (*synth*, *ir*, *pmr*)