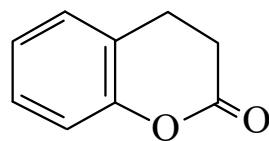




>>Entry Name: 3,4-Dihydro-2H-1-benzopyran-2-one, 9CI

ENTRY UNDER REVIEW

Synonym(s): Hydrocoumarin, 8CI. 3,4-Dihydrocoumarin. 2-Hydroxyhydrocinnamic lactone. 2-Chromanone. Melilotic lactone. Melilotol. **Melilotin**†. Benzodihydropyrone. 2-Oxochroman. FEMA 2381



CAS Registry Number: 119-84-6

Molecular Formula: C₉H₈O₂

Molecular Weight: 148.161

Accurate Mass: 148.05243

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

Biological Source: Isol. from *Melilotus officinalis* and *Artemisia compacta*

Use/Importance: Used as fragrance compd.

Physical Description: Cryst. or liq.

Melting Point: Mp 25°

Boiling Point: Bp 272°. Bp₁₃ 145°

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 1460 mg/kg

Aldrich: W23810-4

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 322A, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1311A, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1386B, (*ir*)
Aldrich Library of NMR Spectra, **7**, 45B, (*pmr*)
Palfray, C.L. *et al.*, *Bull. Soc. Chim. Fr.*, 1938, **5**, 1423, (*synth*)
de Benneville, H. *et al.*, *J.A.C.S.*, 1940, **62**, 283, (*isol*)
Barnes, C.S. *et al.*, *Aust. J. Chem.*, 1964, **17**, 975, (*ms*)
Appleton, R.A. *et al.*, *Phytochemistry*, 1971, **10**, 447, (*isol*)
Morris, W.W., *J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037, (*ir*)
Opdyke, D.L.J., *Food Cosmet. Toxicol.*, 1974, **12**, 521, (*rev, tox*)
Usynina, R.V., *Khim. Prir. Soedin.*, 1976, 810; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, 726, (*isol*)
Chatterjee, A., *Indian J. Chem., Sect. B*, 1977, **15**, 214, (*synth*)
Collins, D.J. *et al.*, *Aust. J. Chem.*, 1989, **42**, 1235, (*synth, cmr*)
Lewis, R.J., *Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HHR500
Pickett, J.E. *et al.*, *Tet. Lett.*, 1992, **33**, 1161, (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 164
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 829-830
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, HHR500