



>>Entry Name: Dodecanal

ENTRY UNDER REVIEW

Synonym(s): Lauric aldehyde. Laurylaldehyde. FEMA 2615

CAS Registry Number: 112-54-9

Type of Compound Code(s): VA0250 WI7900 WI5000 WI2000

$\text{H}_3\text{C}(\text{CH}_2)_{10}\text{CHO}$

Molecular Formula: $\text{C}_{12}\text{H}_{24}\text{O}$

Molecular Weight: 184.321

Accurate Mass: 184.182715

Percentage Composition: C 78.20%; H 13.12%; O 8.68%

Biological Source: Occurs in peel oil from *Chamaecyparis lawsonia*, *Citrus* spp. and kumquat. Also present in ginger coriander, chervil, and scallop and a common component of lepidopteran pheromones

Use/Importance: Perfumery ingredient. Flavouring agent

Physical Description: Cryst.

Melting Point: Mp 44.5°

Boiling Point: Bp₁₀₀ 184-185°. Bp₂₂ 142-143°

Solubility: BERDY SOL: Poorly sol. H_2O

Hazard & Toxicity: Skin and eye irritant. LD₅₀ (rat, orl) 23000 mg/kg

Aldrich: D22200-3

Fluka: 61590

Sigma: D3042

Supelco: 48-2615

>>Derivative: Oxime

Molecular Formula: $\text{C}_{12}\text{H}_{25}\text{NO}$

Molecular Weight: 199.336

Accurate Mass: 199.193614

Percentage Composition: C 72.31%; H 12.64%; N 7.03%; O 8.03%

Melting Point: Mp 73°

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 106°

References:

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 361B, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 469D, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 556B, (ir)

Kraft, F., *Ber.*, 1880, **13**, 1413

Davies, R.R. *et al.*, *J.C.S.*, 1943, 84, (synth)

Ikeda, R.M. *et al.*, *J. Agric. Food Chem.*, 1962, **10**, 98, (isol)

Opdyke, D.L.J., *Food Cosmet. Toxicol.*, 1973, **11**, 483, (rev, tox)

Boss, B.D. *et al.*, *Anal. Chem.*, 1976, **48**, 417, (glc, ms)

Tengoe, J. *et al.*, *Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **55**, 179, (isol)

Lewis, R.J., *Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DXT000

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1542-1543, (occurs, props)

Aurell, M.J. *et al.*, *Tetrahedron*, 1997, **53**, 10883-10898, (synth, pmr)

Sharma, A. *et al.*, *J.O.C.*, 1999, **22**, 8059-8062, (synth, ir, pmr)

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