



>>Entry Name: Decanal, 9CI

ENTRY UNDER REVIEW

Synonym(s): Decyl aldehyde. Capraldehyde. Caprinaldehyde. FEMA 2362

CAS Registry Number: 112-31-2

$\text{H}_3\text{C}(\text{CH}_2)_8\text{CHO}$

Molecular Formula:  $\text{C}_{10}\text{H}_{20}\text{O}$

Molecular Weight: 156.267

Accurate Mass: 156.151415

Percentage Composition: C 76.86%; H 12.90%; O 10.24%

Biological Source: Constit. of Cassia, Neroli and other oils esp. citrus peel oils. Also present in coriander leaf or seed, caviar, roast turkey, roast filbert, green tea, fish oil, hop oil and beer

Use/Importance: Used in perfumery and flavour industries

Physical Description: Liq. with strong orange-peel odour

Melting Point: Mp  $-5$  approx. $^{\circ}$

Boiling Point: Bp  $208-209^{\circ}$ . Bp<sub>7</sub>  $81^{\circ}$

Density:  $d_4^{20}$  0.85

Refractive Index:  $n_D^{20}$  1.4887

Hazard & Toxicity: Skin irritant. LD<sub>50</sub> (rat, orl) 3730 mg/kg

Aldrich: W23620-9

Fluka: 21400

Sigma: D7384

Supelco: 48-2362

>>Derivative: Di-Me acetal

Synonym(s): 1,1-Dimethoxydecane. FEMA 2363

CAS Registry Number: 7779-41-1

Molecular Formula:  $\text{C}_{12}\text{H}_{26}\text{O}_2$

Molecular Weight: 202.336

Accurate Mass: 202.19328

Percentage Composition: C 71.23%; H 12.95%; O 15.81%

Use/Importance: Flavouring ingredient

Physical Description: Liq.

Boiling Point: Bp  $218^{\circ}$

Density:  $d^{15.5}$  0.83

Refractive Index:  $n_D^{24}$  1.4244

#### References:

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

*Aldrich Library of  $^{13}\text{C}$  and  $^1\text{H}$  FT NMR Spectra*, 1992, **1**, 732B, (nmr)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 555C, (ir)

Pickard, K.J., *J.C.S.*, 1913, **103**, 1947

Mathis, C. *et al.*, *Phytochemistry*, 1964, **3**, 377, (isol)

Attaway, J.A. *et al.*, *Phytochemistry*, 1966, **5**, 141, (isol)

Opdyke, D.L.J., *Food Cosmet. Toxicol.*, 1973, **11**, 477, (rev, tox)

Morris, W.W., *J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037, (ir, pmr)

Stanley, J.B. *et al.*, *J. Food Sci.*, 1975, **40**, 1134, (ms)

*Org. Synth.*, 1976, **55**, 84, (synth)

Lewis, R.J., *Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DAG000; DAG200

*Fenaroli's Handbook of Flavor Ingredients*, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 145, (di-Me acetal)

*Encyclopedia of Food and Color Additives*, (ed. Burdock, G.A.), CRC Press, 1997, 772-774, (props, occur, di-Me acetal)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DAG000; DAG200