



>>Entry Name: 2-Pentenal, 9CI

ENTRY UNDER REVIEW

Synonym(s): FEMA 3218

CAS Registry Number: 764-39-6

$\text{H}_3\text{CCH}_2\text{CH}=\text{CHCHO}$

Molecular Formula:  $\text{C}_5\text{H}_8\text{O}$

Molecular Weight: 84.118

Accurate Mass: 84.057515

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Biological Source: Constit. of fruit aromas

>>Variant: (*E*)-form

CAS Registry Number: 1576-87-0

Molecular Formula:  $\text{C}_5\text{H}_8\text{O}$

Molecular Weight: 84.118

Accurate Mass: 84.057515

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Boiling Point:  $\text{Bp}_{160}$  80-81°.  $\text{Bp}_{80}$  62-64°

Aldrich: 26925-5

Fluka: 77003

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Orange-red needles ( $\text{CHCl}_3/\text{MeOH}$ )

Melting Point: Mp 163-165°

>>Derivative: Semicarbazone

Melting Point: Mp 177-178°

>>Variant: (*Z*)-form

CAS Registry Number: 1576-86-9

Molecular Formula:  $\text{C}_5\text{H}_8\text{O}$

Molecular Weight: 84.118

Accurate Mass: 84.057515

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Boiling Point:  $\text{Bp}_{85}$  58-60°

Other Data: Forms 2,4-dinitrophenylhydrazone of (*E*)-form

#### References:

*Aldrich Library of  $^{13}\text{C}$  and  $^1\text{H}$  FT NMR Spectra*, 1992, **1**, 735C, (*nmr*)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 559C, (*ir*)

Prévost, C., *Bull. Soc. Chim. Fr.*, 1944, **11**, 218, (*synth*)

Thomas, D.A. *et al.*, *J.C.S.*, 1965, 2988, (*synth*)

Jaenicke, L. *et al.*, *Chem. Ber.*, 1975, **108**, 225, (*synth*)

Bestmann, H.J. *et al.*, *Chem. Ber.*, 1982, **115**, 161, (*synth*)

*Encyclopedia of Food and Color Additives*, (ed. Burdock, G.A.), CRC Press, 1997, 2118-2119, (*use, occur*)

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