



>>Entry Name: 2-Undecenal, 9CI

ENTRY UNDER REVIEW

Synonym(s): FEMA 3423

CAS Registry Number: 2463-77-6

Extra CAS Registry Numbers(s): 1337-83-3

$\text{H}_3\text{C}(\text{CH}_2)_7\text{CH}=\text{CHCHO}$

Molecular Formula: $\text{C}_{11}\text{H}_{20}\text{O}$

Molecular Weight: 168.278

Accurate Mass: 168.151415

Percentage Composition: C 78.51%; H 11.98%; O 9.51%

>>Variant: (*E*)-form

CAS Registry Number: 53448-07-0

Molecular Formula: $\text{C}_{11}\text{H}_{20}\text{O}$

Molecular Weight: 168.278

Accurate Mass: 168.151415

Percentage Composition: C 78.51%; H 11.98%; O 9.51%

Biological Source: Component of dried/smoked fish aroma. Present in leaf and flower essential oils, and fruit (orange peel and blackberries), butter, chicken and roasted nuts

Physical Description: Liq.

Boiling Point: Bp₂ 88-90°

Aldrich: W34230-0

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Solid

Melting Point: Mp 122.6°

Other Data: Assignment to (*E*)-form is not certain

>>Derivative: Semicarbazone

Physical Description: Solid

Melting Point: Mp 161.5-162.5°

Other Data: Assignment to (*E*)-form is not certain

>>Variant: (*Z*)-form

CAS Registry Number: 71277-05-9

Molecular Formula: $\text{C}_{11}\text{H}_{20}\text{O}$

Molecular Weight: 168.278

Accurate Mass: 168.151415

Percentage Composition: C 78.51%; H 11.98%; O 9.51%

Biological Source: Component of roasted chicken/guinea hen meat and mango aroma

Physical Description: Liq.

Boiling Point: Bp₁₈ 129-131°

References:

Swift, C.E. *et al.*, *J.A.C.S.*, 1949, **71**, 1512, (*synth*)

Bestmann, H.J. *et al.*, *Tet. Lett.*, 1977, 121, (*synth, pmr*)

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

Huang, Y.Z. *et al.*, *J.O.C.*, 1987, **52**, 3558, (*synth, pmr, ms, ir, gc*)

Boelens, M.H. *et al.*, *Perfum. Flavor.*, 1987, **12**, 31; *CA*, **107**, 115390x, (*props*)

Richardson, S.D. *et al.*, *Environ. Toxicol. Chem.*, 1991, **10**, 991; *CA*, **115**, 141892x, (*isol, gc, ms*)

Fortes, C.C. *et al.*, *Synth. Commun.*, 1997, **27**, 3917-3941, (*synth, ir, pmr, cmr, ms*)