



>>Entry Name: 3-Octen-2-one

CAS Registry Number: 1669-44-9



Molecular Formula: C₈H₁₄O

Molecular Weight: 126.198

Accurate Mass: 126.104465

Percentage Composition: C 76.14%; H 11.18%; O 12.68%

Biological Source: Vanilla volatile, mushroom flavour component

>>Variant: (*E*)-form

CAS Registry Number: 18402-82-9

Molecular Formula: C₈H₁₄O

Molecular Weight: 126.198

Accurate Mass: 126.104465

Percentage Composition: C 76.14%; H 11.18%; O 12.68%

Physical Description: Oil

Boiling Point: Bp₅₀ 100°

Aldrich: W34160-6

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 93°

>>Variant: (*Z*)-form

CAS Registry Number: 51193-77-2

Molecular Formula: C₈H₁₄O

Molecular Weight: 126.198

Accurate Mass: 126.104465

Percentage Composition: C 76.14%; H 11.18%; O 12.68%

Physical Description: Oil

Boiling Point: Bp₅₀ 68-69°

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 93°

References:

Heilman, R. *et al.*, *Bull. Soc. Chim. Fr.*, 1957, 119, (*synth, uv, ir*)

Clinet, J.C. *et al.*, *Tet. Lett.*, 1978, 1137, (*synth*)

Beak, P. *et al.*, *J.A.C.S.*, 1980, **102**, 3848, (*synth*)

Grayson, D.H. *et al.*, *J.C.S. Perkin 1*, 1986, 2137, (*synth, ir, pmr*)

Barbero, A. *et al.*, *J.C.S. Perkin 1*, 1995, 1525, (*synth, ir, pmr, ms*)