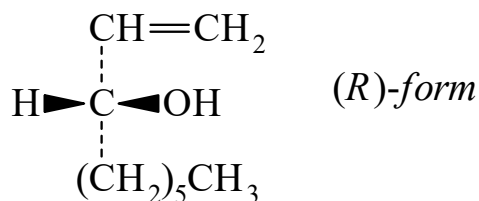




>>Entry Name: 1-Nonen-3-ol, 9CI

ENTRY UNDER REVIEW

Synonym(s): Hexylvinylcarbinol



CAS Registry Number: 21964-44-3

Related CAS Registry Numbers(s): 79646-41-6

Molecular Formula: C₉H₁₈O

Molecular Weight: 142.241

Accurate Mass: 142.135765

Percentage Composition: C 76.00%; H 12.75%; O 11.25%

Biological Source: Isol. from *Petasites japonicus*

Rare Chemicals Library: S43575-9

>>Variant: (R)-form

CAS Registry Number: 79646-41-6

Molecular Formula: C₉H₁₈O

Molecular Weight: 142.241

Accurate Mass: 142.135765

Percentage Composition: C 76.00%; H 12.75%; O 11.25%

Source/Synthesis: Isol. from oil of water fennel *Phellandrium aquaticum*

Optical Rotation: $[\alpha]_{\text{D}}^{25} -17.5$ (c, 1.4 in EtOH) (>95% ee)

>>Variant: (±)-form

CAS Registry Number: 79605-61-1

Molecular Formula: C₉H₁₈O

Molecular Weight: 142.241

Accurate Mass: 142.135765

Percentage Composition: C 76.00%; H 12.75%; O 11.25%

Boiling Point: Bp 193-194°. Bp₂₀ 92.5°

>>Derivative: Ac

CAS Registry Number: 31795-37-6

Molecular Formula: C₁₁H₂₀O₂

Molecular Weight: 184.278

Accurate Mass: 184.14633

Percentage Composition: C 71.70%; H 10.94%; O 17.36%

Biological Source: Constit. of *Petasites japonicus*. Component of Feng Dou Cai

>>Derivative: 4-Nitrobenzoyl

Physical Description: Plates (EtOH)

Melting Point: Mp 36-37°

References:

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Dumont, W. *et al.*, *Angew. Chem., Int. Ed.*, 1974, **13**, 804, (synth)
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Martin, V.S. *et al.*, *J.A.C.S.*, 1981, **103**, 6237, (resoln)
Halazy, S. *et al.*, *Tet. Lett.*, 1981, 2135, (synth)
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Dittmer, D.C. *et al.*, *J.O.C.*, 1993, **58**, 718, (synth, pmr, cmr)