



>>Entry Name: 2-Methyl-3-buten-2-ol

Synonym(s): Isoprenyl alcohol. 1,1-Dimethylallyl alcohol

CAS Registry Number: 115-18-4



Molecular Formula: $\text{C}_5\text{H}_{10}\text{O}$

Molecular Weight: 86.133

Accurate Mass: 86.073165

Percentage Composition: C 69.72%; H 11.70%; O 18.58%

Biological Source: Constit. of ylang-ylang and *Lavandula* oils and hops

Use/Importance: Intermediate in the manuf. of terpene alcohols for perfumery industry

Physical Description: Oil

Boiling Point: Bp 98-99°

Hazard & Toxicity: LD₅₀ (rat, ipr) 1315 mg/kg

Aldrich: W50390-8

Fluka: 66090

Sigma: M8263

>>Derivative: *p*-Nitrobenzoyl

Melting Point: Mp 115-115.5°

>>Derivative: *O*-β-D-Glucopyranoside

Synonym(s): 1,1-Dimethyl-2-propenyl glucoside. 1,1-Dimethylallyl glucoside. **Crenulatin**‡

CAS Registry Number: 63026-02-8

Molecular Formula: $\text{C}_{11}\text{H}_{20}\text{O}_6$

Molecular Weight: 248.275

Accurate Mass: 248.12599

Percentage Composition: C 53.22%; H 8.12%; O 38.67%

Biological Source: Constit. of *Artemisia santolinifolia*, *Ferula loscosii*, *Ferula sinaiaica* and *Rhodiola crenulata*

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 135-136°

Optical Rotation: $[\alpha]_{\text{D}} -25$ (c, 1 in Py)

>>Derivative: *O*-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]

CAS Registry Number: 76873-98-8

Molecular Formula: $\text{C}_{16}\text{H}_{28}\text{O}_{10}$

Molecular Weight: 380.391

Accurate Mass: 380.16825

Percentage Composition: C 50.52%; H 7.42%; O 42.06%

Biological Source: Constit. of *Glehnia littoralis* and *Ligustrum japonicum*

Physical Description: Amorph. powder

Optical Rotation: $[\alpha]_{\text{D}}^{22} -84$ (c, 0.2 in MeOH)

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **1**, 140A, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 210A, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 202C, (*ir*)
Naves, Y.-R. *et al.*, *Bull. Soc. Chim. Fr.*, 1971, 886-888, (*isol*)
Meléndez, E. *et al.*, *An. Quim.*, 1972, **68**, 1283-1294, (*synth*, *pmr*)
Olah, G.A. *et al.*, *J.A.C.S.*, 1975, **97**, 1539-1546, (*cmr*)
Pinar, M.M. *et al.*, *Phytochemistry*, 1977, **16**, 281-282, (*glucoside*)
Jakupovic, J. *et al.*, *Phytochemistry*, 1991, **30**, 1941-1946, (*Crenulatin*)
Ahmed, A.A. *et al.*, *J. Nat. Prod.*, 1996, **59**, 1171-1173, (*glucoside*)
Kitajima, J. *et al.*, *Chem. Pharm. Bull.*, 1998, **46**, 1939-1940, (*apiosylglucoside*)
Vani, P.V.S.N. *et al.*, *Synth. Commun.*, 2001, **31**, 219-224, (*synth*, *pmr*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MHU100