

Product Data Sheet

Product Name: Methyl Salicylate-d₄

Cat. No.: GC91887

Chemical Properties

Cas. No. 1219802-12-6

Chemical Name methyl 2-hydroxybenzoate-3,4,5,6-d₄

SMILES COC(=C(C([2H])=C([2H])C([2H])=C1[2H])O)=O

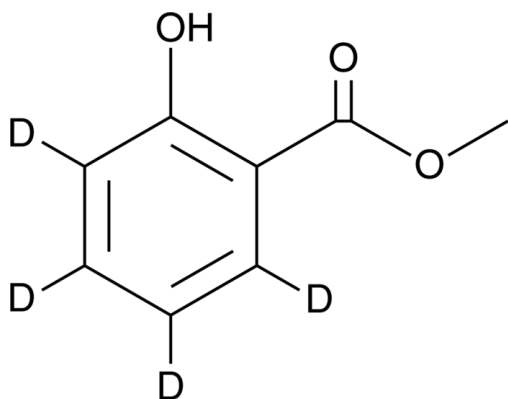
Formula C₈H₄D₄O₃ M.Wt 156.2

Solubility Methyl Acetate: Sparingly soluble: 1-10 mg/ml Storage -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure



Background

Methyl salicylate-d₄ is intended for use as an internal standard for the quantification of methyl salicylate by GC- or LC-MS. Methyl salicylate is a phenol that has been found in *Narcissus* and has diverse biological activities.^{1,2,3,4,5} It scavenges free radicals in a Trolox equivalent antioxidant capacity (TEAC) assay (IC₅₀ = 0.27 μM).² Methyl salicylate (10 mg/ml) is active against *E. coli* and

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S. aureus.³ It activates transient receptor potential ankyrin 1 (Trpa1) and Trp vanilloid 1 (Trpv1) in CHO cells expressing mouse Trpa1 or rat Trpv1 when used at concentrations of 0.6 and 2 mM, respectively.⁴ Methyl salicylate does not induce gastric ulcers in cold-stressed rats and inhibits carrageenan-induced paw edema ($ED_{50} = 220$ mg/kg) and yeast-induced fever in rats.⁵

Formulations containing methyl salicylate have been used as topical analgesics, oral antiseptics, and food additives.

References:

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- [2]. Battino, M., Ferreiro, M.S., Fattorini, D., et al. In vitro antioxidant activities of mouthrinses and their components. *J. Clin. Periodontol.* 29(5)462-467(2002).
- [3]. Khiati, Z., and Othman, A.A. Synthesis and antibacterial activity of 1,3,4-oxadiazole and 1,2,4-triazole derivatives of salicylic acid and its synthetic intermediates. *S. Afr. J. Chem.* 6020-24(2007).
- [4]. Bandell, M., Story, G.M., Hwang, S.W., et al. Noxious cold ion channel TRPA1 is activated by pungent compounds and bradykinin. *Neuron* 41(6)849-857(2004).
- [5]. Rainsford, K.D., and Whitehouse, M.W. Anti-inflammatory/anti-pyretic salicylic acid esters with low gastric ulcerogenic activity. *Agents Actions* 10(5)451-456(1980).

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