

PRODUCT INFORMATION



6',7'-Epoxybergamottin

Item No. 19760

CAS Registry No.: 206978-14-5
Formal Name: 4-[[[(2E)-5-(3,3-dimethyl-2-oxiranyl)-3-methyl-2-penten-1-yl]oxy]-7H-furo[3,2-g][1]benzopyran-7-one

Synonym: Epoxybergamottin

MF: C₂₁H₂₂O₅

FW: 354.4

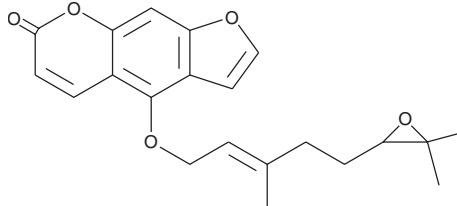
Purity: ≥95%

UV/Vis.: λ_{max}: 251, 311 nm

Supplied as: A crystalline solid

Storage: -20°C

Stability: ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

6',7'-Epoxybergamottin is supplied as a crystalline solid. A stock solution may be made by dissolving the 6',7'-epoxybergamottin in the solvent of choice, which should be purged with an inert gas. 6',7'-Epoxybergamottin is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of 6',7'-epoxybergamottin in ethanol is approximately 10 mg/ml and approximately 30 mg/ml in DMSO and DMF.

6',7'-Epoxybergamottin is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, 6',7'-epoxybergamottin should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. 6',7'-Epoxybergamottin has a solubility of approximately 0.50 mg/ml in a 1:1 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

6',7'-Epoxybergamottin is a furanocoumarin found in grapefruit.¹ It is a potent inhibitor of the cytochrome P450 (CYP) isoform CYP3A4 with an IC₅₀ value of 0.30 ppm in a cell-free assay, 0.33 μM in HL7 human liver cells, and 0.22 μM in S9 human intestine cells.² It has been studied in the context of drug interactions with grapefruit constituents. It is found in grapefruit juice at concentrations of 0.1-7.4 μM and inhibits the transport of talinolol (Item No. 16116), a permeability glycoprotein (P-gp/ABCB1) transporter substrate, across Caco-2 cell monolayers (IC₅₀ = 0.7 μM).³

References

1. Manthey, J.A., Myung, K., Mertens-Talcott, S., *et al. Proc. Fla. State Hort. Soc.* **119(1)**, 361-366 (2006).
2. Row, E.C., Brown, S.A., Stachulski, A.V., *et al. Org. Biomol. Chem.* **4(8)**, 1604-1610 (2006).
3. de Castro, W.V., Mertens-Talcott, S., Derendorf, H., *et al. J. Pharm. Sci.* **96(10)**, 2808-2817 (2007).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the [complete](#) Safety Data Sheet, which has been sent via email to your institution.

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