



Formula: C<sub>21</sub>H<sub>22</sub>O<sub>4</sub>

MW: 338.4

CAS: 7380-40

MDL: MFCD06668139

TNP: TNP00285

BERGAMOTTIN; BERGAPTIN; BERGAMOTIN; BERGAMOTINE; AKOS 214-13;  
5-GERANYLOXYPSORALEN; 4-GERANYLOXYPSORALEN; GF-I-2



LogP: 5.36

LogS: -4.7

Acceptors: 4

Donors: 0

Rotation Bonds: 6

Chiral Centers: 0

N+O: 4

LIPINSKY: 4

IUPAC: 5-((2Z)-3,7-dimethylocta-2,6-dienyloxy)furano[3,2-g]chromen-2-one

Smiles: c12c(oc(cc2)=O)cc2c(c1OCC=C(/CCC=C(/C)C)C)cco2

Specification: Miscellaneous; Coumarins Bergamotone Chemical Properties:

mp 75-80 C storage temp. 2-8C Safety 22-24/25 WGK Germany 3 F 10-23 Bergamotone

Usage And Synthesis Bergamotine