

5-geranyloxy-7-methoxycoumarin

Inchi:	InChI=1S/C21H26O3/c1-15(2)7-5-8-16(3)9-6-10-17-13-18(23-4)14-20-19(17)11-12-21(22)
InchiKey:	QWPLVRCHBYSUDX-CXUHLZMHTA-N
Formula:	C21H26O3
SMILES:	COc1cc(CCC=C(C)CCG=C(C)C)c2ccc(=O)oc2c1
Mol. weight [g/mol]:	326.43
CAS:	7380-39-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.83		Crippen Method
logp	5.427		Crippen Method
mcvol	272.540	ml/mol	McGowan Method
rinsol	2862.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7380394&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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