

4-(2,3-Dihydroxy-3-methylbutoxy)furo(3,2-g)chromen-7-one

Other names:	Oxypeucedanin hydrate
Inchi:	InChI=1S/C16H16O6/c1-16(2,19)13(17)8-21-15-9-3-4-14(18)22-12(9)7-11-10(15)5-6-20
InchiKey:	PEWFWDOPJISUOK-UHFFFAOYSA-N
Formula:	C16H16O6
SMILES:	CC(C)(O)C(O)COc1c2ccoc2cc2oc(=O)ccc12
Mol. weight [g/mol]:	304.29
CAS:	24724-52-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.52		Crippen Method
logp	2.050		Crippen Method
mcvol	213.140	ml/mol	McGowan Method
rinpola	2765.10		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24724525&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpola:	Non-polar retention indices

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