

Oxypeucedanin

Inchi:	InChI=1S/C16H14O5/c1-16(2)13(21-16)8-19-15-9-3-4-14(17)20-12(9)7-11-10(15)5-6-18-
InchiKey:	QTAGQHZOLRFCBU-UHFFFAOYSA-N
Formula:	C16H14O5
SMILES:	CC1(C)OC1COc1c2ccoc2cc2oc(=O)ccc12
Mol. weight [g/mol]:	286.28
CAS:	737-52-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.97		Crippen Method
logp	3.095		Crippen Method
mcvol	196.410	ml/mol	McGowan Method
rinpol	2500.70		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C737520&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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<https://www.chemeo.com/cid/82-212-5/Oxypeucedanin.pdf>

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