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
rinpol	2500.70		NIST Webbook

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