oxypeucedanin methanolate

Inchi: InChI=1S/C17H18O6/c1-17(2,20-3)14(18)9-22-16-10-4-5-15(19)23-13(10)8-12-11(16)6-7
InchiKey: UHENVVIVPZCJOA-UHFFFAOYSA-N
Formula: C17H18O6
SMILES: COC(C)(C)C(O)COc1c2ccoc2cc2oc(=O)ccc12
Mol. weight [g/mol]: 318.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.76		Crippen Method
logp	2.704		Crippen Method
mcvol	227.230	ml/mol	McGowan Method
rinpol	2760.00		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=R422416&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