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-CYBMUJFWSA-N
Formula: C16H16O6
SMILES: CC(C)(O)C(O)COc1c2ccoc2cc2oc(=O)ccc12
Mol. weight [g/mol]: 304.29
CAS: 2643-85-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.52		Crippen Method
logp	2.050		Crippen Method
mcvol	213.140	ml/mol	McGowan Method
rinpol	2739.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2643858&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.