pabulenol

Inchi: InChI=1S/C16H14O5/c1-9(2)12(17)8-20-16-10-3-4-15(18)21-14(10)7-13-11(16)5-6-19-13
InchiKey: BVMOMQJYQYBMKL-GFCCVEGCSA-N
Formula: C16H14O5
SMILES: C=C(C)C(O)COc1c2ccoc2cc2oc(=O)ccc12
Mol. weight [g/mol]: 286.28
CAS: 33889-70-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.99		Crippen Method
logp	2.855		Crippen Method
mcvol	202.970	ml/mol	McGowan Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33889702&Units=SI

Legend

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