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

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https://www.chemeo.com/cid/64-276-5/pabulenol.pdf

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