

heraclenol

Inchi: InChI=1S/C16H16O6/c1-16(2,19)11(17)8-21-15-13-10(5-6-20-13)7-9-3-4-12(18)22-14(9)
InchiKey: FOINLJRVEBYARJ-LLVKDONJSA-N
Formula: C16H16O6
SMILES: CC(C)(O)C(O)COc1c2occc2cc2ccc(=O)oc12
Mol. weight [g/mol]: 304.29
CAS: 31575-93-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.52		Crippen Method
logp	2.050		Crippen Method
mcvol	213.140	ml/mol	McGowan Method
rinpola	2670.00		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=C31575936&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
rinpola: Non-polar retention indices

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<https://www.chemeo.com/cid/37-806-6/heraclenol.pdf>

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