

marmin

Inchi: InChI=1S/C19H24O5/c1-13(4-8-17(20)19(2,3)22)10-11-23-15-7-5-14-6-9-18(21)24-16(14)
InchiKey: QYYKWTUUCOTGNS-RTGRKSDTSA-N
Formula: C19H24O5
SMILES: CC(=CCOc1ccc2ccc(=O)oc2c1)CCC(O)C(C)(C)O
Mol. weight [g/mol]: 332.39
CAS: 14957-38-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.92		Crippen Method
logp	3.030		Crippen Method
mcvol	260.400	ml/mol	McGowan Method
rinpola	2985.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C14957381&Units=SI>
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>

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/56-894-8/marmin.pdf>

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