

Mucronatine

Inchi: InChI=1S/C19H27NO5/c1-4-13-10-12(3)19(23,5-2)18(22)24-11-14-6-8-20-9-7-15(16(14))
InchiKey: FPRDBFWVOJWDMI-GFGUIIKYSA-N
Formula: C19H27NO5
SMILES: CC=C1CC(C)C(O)(CC)C(=O)OCC2=CCN3CCC(OC1=O)C23
Mol. weight [g/mol]: 349.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	1.583		Crippen Method
mcvol	268.120	ml/mol	McGowan Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R422718&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/35-476-5/Mucronatine.pdf>

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