

Rinderine

Inchi: InChI=1S/C15H27NO5/c1-9(2)15(20,10(3)17)14(19)21-8-11-4-6-16-7-5-12(18)13(11)16/
InchiKey: NMPPLGMVCCNRTJ-UHFFFAOYSA-N
Formula: C15H27NO5
SMILES: CC(C)C(O)(C(=O)OCC1CCN2CCC(O)C12)C(C)O
Mol. weight [g/mol]: 301.38
CAS: 6029-84-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.08		Crippen Method
logp	-0.247		Crippen Method
mcvol	235.520	ml/mol	McGowan Method
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2153.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2152.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6029841&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/57-868-6/Rinderine.pdf>

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