

Retrorcine

Inchi: InChI=1S/C18H25NO6/c1-3-12-8-11(2)18(23,10-20)17(22)24-9-13-4-6-19-7-5-14(15(13))
InchiKey: BCJMNZRQJAVDLD-OQIMHWJESA-N
Formula: C18H25NO6
SMILES: CC=C1CC(C)C(O)(CO)C(=O)OCC2=CCN3CCC(OC1=O)C23
Mol. weight [g/mol]: 351.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	0.165		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
rinpol	2585.00		NIST Webbook
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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=R636645&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/76-832-4/Retrorcine.pdf>

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