

Phygrine

Inchi: InChI=1S/C16H28N2O2/c1-12(19)9-14-6-7-15(18(14)3)11-16(20)10-13-5-4-8-17(13)2/h1
InchiKey: UBFAEXSSMSJTQV-ZYOSVBKOSA-N
Formula: C16H28N2O2
SMILES: CC(=O)CC1CCC(CC(=O)CC2CCCN2C)N1C
Mol. weight [g/mol]: 280.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	1.872		Crippen Method
mcvol	237.680	ml/mol	McGowan Method
rinpol	2045.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2045.00		NIST Webbook
rinpol	2043.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R510182&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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

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