Prajmaline

Inchi: InChI=1S/C23H32N2O2/c1-4-10-25-18-11-15(14(5-2)13-26)20-19(25)12-23(22(20)27)16
InchiKey: FNVKGPJJWIKOEY-XFHIVPIVSA-N
Formula: C23H32N2O2
SMILES: CCCN1C2CC34c5ccccc5N(C)C3C1CC(C(C=O)CC)C2C4O
Mol. weight [g/mol]: 368.51
CAS: 35080-11-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	2.831		Crippen Method
mcvol	295.130	ml/mol	McGowan Method
rinpol	2887.00		NIST Webbook
rinpol	2925.00		NIST Webbook
rinpol	2925.00		NIST Webbook

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=C35080116&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

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https://www.chemeo.com/cid/50-953-8/Prajmaline.pdf

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