Ibogaine

Other names:	Ibogamine, 12-methoxy- (-)-Ibogaine 6,9-Methano-5H-pyrido[1',2':1,2]azepino[4,5-b]indole, ibogamine deriv. Ibogain 12-methoxyibogamine
Inchi:	InChI=1S/C20H26N2O/c1-3-13-8-12-9-17-19-15(6-7-22(11-12)20(13)17)16-10-14(23-2)4
InchiKey:	HSIBGVUMFOSJPD-UHFFFAOYSA-N
Formula:	C20H26N2O
SMILES:	CCC1CC2CC3c4[nH]c5ccc(OC)cc5c4CCN(C2)C13
Mol. weight [g/mol]:	310.43
CAS:	83-74-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	3.455		Crippen Method
mcvol	246.990	ml/mol	McGowan Method
rinpol	2895.00		NIST Webbook
rinpol	2915.00		NIST Webbook
rinpol	2900.00		NIST Webbook
rinpol	2895.00		NIST Webbook
rinpol	2872.00		NIST Webbook
rinpol	2908.00		NIST Webbook
rinpol	2900.00		NIST Webbook
rinpol	2872.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83749&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/97-874-5/Ibogaine.pdf
Generated by Cheméo on 2024-04-20 09:06:57.164326148 +0000 UTC m=+15893266.084903463.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.