

oroboidine

Inchi:	InChI=1S/C20H27N3O3/c24-19-5-1-4-17-13-9-14(12-23(17)19)18-10-15(6-8-22(18)11-13
InchiKey:	YFRYJFMFQOBOSY-SYQKBPBVSA-N
Formula:	C20H27N3O3
SMILES:	O=C(OC1CCN2CC3CC(CN4C(=O)CCCC34)C2C1)c1ccc[nH]1
Mol. weight [g/mol]:	357.45
CAS:	6874-80-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	1.553		Crippen Method
mcvol	268.710	ml/mol	McGowan Method
rinpol	3050.00		NIST Webbook
rinpol	3050.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6874802&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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<https://www.chemeo.com/cid/10-952-3/oroboidine.pdf>

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