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