Quebrachamine

Other names:	2H-3,7-Methanoazacycloundecino[5,4-b]indole, 7-ethyl-1,4,5,6,7,8,9,10-octahydro-, (R)- 2H-3,7-Methanoazacycloundecino[5,4-b]indole, 7-ethyl-1,4,5,6,7,8,9,10-octahydro-, (-)- Kamassine Quebrachamin 2H-3,7-Methanoazacycloundecino[5,4-b]indole, 7-ethyl-1,4,5,6,7,8,9
Inchi:	InChI=1S/C19H26N2/c1-2-19-10-5-12-21(14-19)13-9-16-15-6-3-4-7-17(15)20-18(16)8-11
InchiKey:	FDNDLNFGITWTOZ-IBGZPJMESA-N
Formula:	C19H26N2
SMILES:	CCC12CCCN(CCc3c([nH]c4ccccc34)CC1)C2
Mol. weight [g/mol]:	282.42
CAS:	4850-21-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.15		Crippen Method
logp	3.667		Crippen Method
mcvol	237.890	ml/mol	McGowan Method
rinpol	498.03		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4850219&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