Mebhydrolin

Other names:	3-Benzyl-6-methyl-1,2,3,4-tetrahydro-«gamma»-carboline
	1H-Pyrido[4,3-b]indole, 2,3,4,5-tetrahydro-2-methyl-5-(phenylmethyl)-
	5-Benzyl-1,3,4,5-tetrahydro-2-methyl-2H-pyrido[4,3-b]indole
	Incidal
	Mebhydroline
Inchi:	InChI=1S/C19H20N2/c1-20-12-11-19-17(14-20)16-9-5-6-10-18(16)21(19)13-15-7-3-2-4-8
InchiKey:	FQQIIPAOSKSOJM-UHFFFAOYSA-N
Formula:	C19H20N2
SMILES:	CN1CCc2c(c3ccccc3n2Cc2ccccc2)C1
Mol. weight [g/mol]:	276.38
CAS:	524-81-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	3.678		Crippen Method
mcvol	224.990	ml/mol	McGowan Method
rinpol	2476.00		NIST Webbook
rinpol	2449.00		NIST Webbook
rinpol	2449.00		NIST Webbook
rinpol	2450.00		NIST Webbook
rinpol	2465.00		NIST Webbook
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C524812&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