Nomifensine

Other names:	Isoquinoline, 1,2,3,4-tetrahydro-8-amino-2-methyl-4-phenyl- 8-Amino-2-methyl-4-phenyl-1,2,3,4-tetrahydroisoquinoline 8-Isoquinolinamine, 1,2,3,4-tetrahydro-2-methyl-4-phenyl- Nomifensin 8-Amino-1,2,3,4-tetrahydro-2-methyl-4-phenylisoquinoline 2-Methyl-4-phenyl-1,2,3,4-tetrahydro-8-isoquinolinamine Linamiphen Nomiphensine Nomifenison
Inchi:	InChI=1S/C16H18N2/c1-18-10-14(12-6-3-2-4-7-12)13-8-5-9-16(17)15(13)11-18/h2-9,14H
InchiKey:	XXPANQJNYNUNES-UHFFFAOYSA-N
Formula:	C16H18N2
SMILES:	CN1Cc2c(N)cccc2C(c2ccccc2)C1
Mol. weight [g/mol]:	238.33
CAS:	24526-64-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.35		Crippen Method
logp	2.846		Crippen Method
mcvol	197.880	ml/mol	McGowan Method
rinpol	2122.00		NIST Webbook
rinpol	2124.00		NIST Webbook
rinpol	2108.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24526645&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices