

Nomifensine acetate

Other names:	Nomifensine, acetylated
Inchi:	InChI=1S/C18H20N2O/c1-13(21)19-18-10-6-9-15-16(11-20(2)12-17(15)18)14-7-4-3-5-8-
InchiKey:	UJROOBEEKKHHV-UHFFFAOYSA-N
Formula:	C18H20N2O
SMILES:	CC(O)=Nc1cccc2c1CN(C)CC2c1cccc1
Mol. weight [g/mol]:	280.36
CAS:	63806-80-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.10		Crippen Method
logp	3.872		Crippen Method
mcvol	227.630	ml/mol	McGowan Method
rinpol	2470.00		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=C63806804&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

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<https://www.chemeo.com/cid/97-523-4/Nomifensine-acetate.pdf>

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