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: UJROOBBEEKKHHV-UHFFFAOYSA-N
Formula: C18H20N2O
SMILES: CC(O)=Nc1cccc2c1CN(C)CC2c1ccccc1
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