Nomifensine M(HO-methoxy), diacetylated

Inchi: InChI=1S/C21H24N2O4/c1-13(24)22-21-17-12-23(3)11-16(15-8-6-5-7-9-15)20(17)18(27-
InchiKey: VRHQHHTYSZOVRA-UHFFFAOYSA-N
Formula: C21H24N2O4
SMILES: COc1cc(OC(C)=O)c2c(c1NC(C)=O)CN(C)CC2c1ccccc1
Mol. weight [g/mol]: 368.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.35		Crippen Method
logp	3.156		Crippen Method
mcvol	283.210	ml/mol	McGowan Method
rinpol	2970.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R311123&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