Nomifensine M(HO), diacetylated, isomer # 1

Inchi: InChI=1S/C20H22N2O3/c1-13(23)21-18-9-10-19(25-14(2)24)20-16(11-22(3)12-17(18)20
InchiKey: ZZHMFLCUNJFKJE-UHFFFAOYSA-N
Formula: C20H22N2O3
SMILES: CC(=O)Nc1ccc(OC(C)=O)c2c1CN(C)CC2c1ccccc1
Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Crippen Method
logp	3.148		Crippen Method
mcvol	263.250	ml/mol	McGowan Method
rinpol	2850.00		NIST Webbook

Sources

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=R311118&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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