

Nomifemsine M(HO), diacetylated, isomer # 2

Inchi: InChI=1S/C20H22N2O3/c1-13(23)21-20-18-12-22(3)11-17(15-7-5-4-6-8-15)16(18)9-10-1
InchiKey: XXVHJDYSAUNKQM-UHFFFAOYSA-N
Formula: C20H22N2O3
SMILES: CC(=O)Nc1c(OC(C)=O)ccc2c1CN(C)CC2c1cccc1
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	2880.00		NIST Webbook
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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=R311094&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

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<https://www.chemeo.com/cid/31-332-8/Nomifemsine-M-HO-diacetylated-isomer-2.pdf>

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