Nefazodone-M (N-desalkyl-HO-) isomer-2 2AC

Inchi: InChI=1S/C14H17ClN2O3/c1-10(18)16-5-7-17(8-6-16)13-9-12(15)3-4-14(13)20-11(2)19/
InchiKey: VWFXCVSFQAAADM-UHFFFAOYSA-N
Formula: C14H17ClN2O3
SMILES: CC(=O)Oc1ccc(Cl)cc1N1CCN(C(C)=O)CC1
Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.29		Crippen Method
logp	1.934		Crippen Method
mcvol	214.710	ml/mol	McGowan Method
rinpol	2355.00		NIST Webbook
rinpol	2355.00		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=R331147&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.