Nefazodone-M (desamino-HO-) AC

Inchi: InChI=1S/C17H23N3O4/c1-3-16-18-20(10-7-12-23-14(2)21)17(22)19(16)11-13-24-15-8-5
InchiKey: IDEVITANEQDECY-UHFFFAOYSA-N
Formula: C17H23N3O4
SMILES: CCc1nn(CCCOC(C)=O)c(=O)n1CCOc1ccccc1
Mol. weight [g/mol]: 333.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	1.639		Crippen Method
mcvol	256.290	ml/mol	McGowan Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R331107&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

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