

Nefazodone-M (HO-ethyl-desamino-HO-) AC

Inchi:	InChI=1S/C19H25N3O6/c1-14(28-16(3)24)18-20-22(10-7-12-26-15(2)23)19(25)21(18)11
InchiKey:	SHODBRRFZSWYJQ-UHFFFAOYSA-N
Formula:	C19H25N3O6
SMILES:	CC(=O)OCCCN1nc(C(C)OC(C)=O)n(CCOc2ccccc2)c1=O
Mol. weight [g/mol]:	391.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	1.701		Crippen Method
mcvol	291.910	ml/mol	McGowan Method
rinpola	2645.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R331112&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
rinpola:	Non-polar retention indices

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<https://www.chemeo.com/cid/25-488-3/Nefazodone-M-HO-ethyl-desamino-HO-AC.pdf>

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