

# Trazodone-M (desamino-HO-) AC

<b>Inchi:</b>	InChI=1S/C11H13N3O3/c1-9(15)17-8-4-7-14-11(16)13-6-3-2-5-10(13)12-14/h2-3,5-6H,4
<b>InchiKey:</b>	IBSOHHYNSTVJTL-UHFFFAOYSA-N
<b>Formula:</b>	C11H13N3O3
<b>SMILES:</b>	CC(=O)OCCCN1nc2ccccc2c1=O
<b>Mol. weight [g/mol]:</b>	235.24

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	0.449		Crippen Method
mcvol	170.180	ml/mol	McGowan Method
rinpola	1985.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R331172&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R331172&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

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

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