

# N-Desmethyldomipramine ac.

<b>Other names:</b>	Domipramine M(Nor), acetylated
<b>Inchi:</b>	InChI=1S/C20H23ClN2O/c1-15(24)22(2)12-5-13-23-19-7-4-3-6-16(19)8-9-17-10-11-18(2)
<b>InchiKey:</b>	MKZYWCOSALTCPB-UHFFFAOYSA-N
<b>Formula:</b>	C20H23ClN2O
<b>SMILES:</b>	CC(=O)N(C)CCCN1c2ccccc2CCc2ccc(Cl)cc21
<b>Mol. weight [g/mol]:</b>	342.86
<b>CAS:</b>	72103-49-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.96		Crippen Method
logp	4.445		Crippen Method
mcvol	268.050	ml/mol	McGowan Method
rinpol	2994.00		NIST Webbook
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## 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=C72103492&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C72103492&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>rinpol:</b>	Non-polar retention indices

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