

# Maprotiline, N-acetyl-

<b>Other names:</b>	Maprotiline, acetylated
<b>Inchi:</b>	InChI=1S/C22H25NO/c1-16(24)23(2)15-7-13-22-14-12-17(18-8-3-5-10-20(18)22)19-9-4-
<b>InchiKey:</b>	IPDIKPLOBPRIPB-UHFFFAOYSA-N
<b>Formula:</b>	C22H25NO
<b>SMILES:</b>	CC(=O)N(C)CCCC12CCC(c3ccccc31)c1cccc12
<b>Mol. weight [g/mol]:</b>	319.44
<b>CAS:</b>	78508-60-8

## Physical Properties

Property code	Value	Unit	Source
gf	461.99	kJ/mol	Joback Method
hf	80.82	kJ/mol	Joback Method
hfus	38.83	kJ/mol	Joback Method
hvap	77.56	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.470		Crippen Method
mcvol	263.150	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	837.57	K	Joback Method
tc	1069.51	K	Joback Method
tf	564.80	K	Joback Method
vc	1.004	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.06	J/molxK	837.57	Joback Method
cpg	840.16	J/molxK	876.23	Joback Method
cpg	859.07	J/molxK	914.88	Joback Method
cpg	878.09	J/molxK	953.54	Joback Method
cpg	897.50	J/molxK	992.20	Joback Method
cpg	917.60	J/molxK	1030.85	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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=C78508608&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C78508608&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<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>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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