

# Maprotiline M(Nor), acetyl conjugate

<b>Inchi:</b>	InChI=1S/C21H23NO/c1-15(23)22-14-6-12-21-13-11-16(17-7-2-4-9-19(17)21)18-8-3-5-1
<b>InchiKey:</b>	XEWCNCFSWLDCFU-UHFFFAOYSA-N
<b>Formula:</b>	C21H23NO
<b>SMILES:</b>	CC(=O)NCCCC12CCC(c3ccccc31)c1cccc12
<b>Mol. weight [g/mol]:</b>	305.41

## Physical Properties

Property code	Value	Unit	Source
gf	432.18	kJ/mol	Joback Method
hf	87.40	kJ/mol	Joback Method
hfus	38.32	kJ/mol	Joback Method
hvap	79.73	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.128		Crippen Method
mvol	249.060	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	2765.00		NIST Webbook
tb	852.42	K	Joback Method
tc	1089.24	K	Joback Method
tf	573.72	K	Joback Method
vc	0.965	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.17	J/mol×K	852.42	Joback Method
cpg	797.59	J/mol×K	891.89	Joback Method
cpg	815.97	J/mol×K	931.36	Joback Method
cpg	834.63	J/mol×K	970.83	Joback Method
cpg	853.85	J/mol×K	1010.30	Joback Method
cpg	873.93	J/mol×K	1049.77	Joback Method
cpg	895.16	J/mol×K	1089.24	Joback Method

# Sources

<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=R311014&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R311014&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>rinpola:</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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