

# Maprotiline M(di-HO), diacetylated

<b>Inchi:</b>	InChI=1S/C24H27NO4/c1-15(26)25(3)12-4-10-24-11-9-19(20-7-5-17(28)13-22(20)24)21-
<b>InchiKey:</b>	DFNVBHIKRFICNK-UHFFFAOYSA-N
<b>Formula:</b>	C24H27NO4
<b>SMILES:</b>	CC(=O)Oc1ccc2c(c1)C1(CCCN(C)C(C)=O)CCC2c2ccc(O)cc21
<b>Mol. weight [g/mol]:</b>	393.48

## Physical Properties

Property code	Value	Unit	Source
gf	80.66	kJ/mol	Joback Method
hf	-394.04	kJ/mol	Joback Method
hfus	52.19	kJ/mol	Joback Method
hvap	104.85	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.101		Crippen Method
mvol	304.640	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook
tb	1045.22	K	Joback Method
tc	1289.34	K	Joback Method
tf	783.74	K	Joback Method
vc	1.105	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.24	J/mol×K	1045.22	Joback Method
cpg	1083.65	J/mol×K	1085.91	Joback Method
cpg	1110.77	J/mol×K	1126.59	Joback Method
cpg	1139.97	J/mol×K	1167.28	Joback Method
cpg	1171.62	J/mol×K	1207.97	Joback Method
cpg	1206.08	J/mol×K	1248.66	Joback Method
cpg	1243.71	J/mol×K	1289.34	Joback Method

# 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>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=R310977&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R310977&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>

# 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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