

# Zotepine-M (nor-/bis-nor-) HYAC

<b>Inchi:</b>	InChI=1S/C16H11ClO3S/c1-9(18)20-12-3-5-15-10(6-12)7-14(19)13-8-11(17)2-4-16(13)2
<b>InchiKey:</b>	QTSRSLWUVSULNG-UHFFFAOYSA-N
<b>Formula:</b>	C16H11ClO3S
<b>SMILES:</b>	CC(=O)Oc1ccc2c(c1)CC(=O)c1cc(Cl)ccc1S2
<b>Mol. weight [g/mol]:</b>	318.77

## Physical Properties

Property code	Value	Unit	Source
gf	10.02	kJ/mol	Joback Method
hf	-206.23	kJ/mol	Joback Method
hfus	30.94	kJ/mol	Joback Method
hvap	82.23	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.155		Crippen Method
mvol	215.520	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rmpol	2440.00		NIST Webbook
rmpol	2440.00		NIST Webbook
tb	879.54	K	Joback Method
tc	1149.86	K	Joback Method
tf	648.93	K	Joback Method
vc	0.799	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.43	J/mol×K	879.54	Joback Method
cpg	593.11	J/mol×K	924.59	Joback Method
cpg	603.54	J/mol×K	969.65	Joback Method
cpg	612.79	J/mol×K	1014.70	Joback Method
cpg	620.89	J/mol×K	1059.75	Joback Method
cpg	627.91	J/mol×K	1104.80	Joback Method
cpg	633.91	J/mol×K	1149.86	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=R331330&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R331330&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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