

# Dosulepin-M (bis-nor-) AC

<b>Inchi:</b>	InChI=1S/C19H19NOS/c1-14(21)20-12-6-10-17-16-8-3-2-7-15(16)13-22-19-11-5-4-9-18(
<b>InchiKey:</b>	PFUSITCDPXGKEZ-YVLHZVERSA-N
<b>Formula:</b>	C19H19NOS
<b>SMILES:</b>	CC(=O)NCCC=C1c2ccccc2CSc2ccccc21
<b>Mol. weight [g/mol]:</b>	309.43

## Physical Properties

Property code	Value	Unit	Source
gf	428.91	kJ/mol	Joback Method
hf	169.95	kJ/mol	Joback Method
hfus	40.01	kJ/mol	Joback Method
hvap	83.77	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.250		Crippen Method
mcvol	243.790	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinqol	2800.00		NIST Webbook
tb	867.36	K	Joback Method
tc	1117.26	K	Joback Method
tf	600.35	K	Joback Method
vc	0.911	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.59	J/molxK	867.36	Joback Method
cpg	719.08	J/molxK	909.01	Joback Method
cpg	732.65	J/molxK	950.66	Joback Method
cpg	745.47	J/molxK	992.31	Joback Method
cpg	757.68	J/molxK	1033.96	Joback Method
cpg	769.43	J/molxK	1075.61	Joback Method
cpg	780.89	J/molxK	1117.26	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=R331003&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R331003&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.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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