

# Sotalol - H2O, acetylated

<b>Inchi:</b>	InChI=1S/C14H20N2O3S/c1-11(2)16(12(3)17)10-9-13-5-7-14(8-6-13)15-20(4,18)19/h5-1
<b>InchiKey:</b>	WSFZELQFQMNUKA-MDZDMXLPSA-N
<b>Formula:</b>	C14H20N2O3S
<b>SMILES:</b>	CC(=O)N(C=Cc1ccc(NS(C)(=O)=O)cc1)C(C)C
<b>Mol. weight [g/mol]:</b>	296.38

## Physical Properties

Property code	Value	Unit	Source
gf	-149.73	kJ/mol	Joback Method
hf	-440.22	kJ/mol	Joback Method
hfus	43.44	kJ/mol	Joback Method
hvap	83.13	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.286		Crippen Method
mcvol	229.680	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
rinsol	2675.00		NIST Webbook
tb	719.36	K	Joback Method
tc	924.91	K	Joback Method
tf	440.02	K	Joback Method
vc	0.871	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.37	J/molxK	719.36	Joback Method
cpg	643.52	J/molxK	753.62	Joback Method
cpg	657.59	J/molxK	787.88	Joback Method
cpg	670.62	J/molxK	822.14	Joback Method
cpg	682.64	J/molxK	856.39	Joback Method
cpg	693.72	J/molxK	890.65	Joback Method
cpg	703.88	J/molxK	924.91	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=R583036&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R583036&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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