

# allicin

<b>Inchi:</b>	InChI=1S/C6H10OS2/c1-3-5-8-9(7)6-4-2/h3-4H,1-2,5-6H2
<b>InchiKey:</b>	JDLKFOPOAOFWQN-UHFFFAOYSA-N
<b>Formula:</b>	C6H10OS2
<b>SMILES:</b>	C=CCSS(=O)CC=C
<b>Mol. weight [g/mol]:</b>	162.28

## Physical Properties

Property code	Value	Unit	Source
gf	-9.27	kJ/mol	Joback Method
hf	-80.18	kJ/mol	Joback Method
hfus	20.62	kJ/mol	Joback Method
hvap	47.15	kJ/mol	Joback Method
log10ws	-0.83		Aqueous Solubility Prediction Method
log10ws	-0.83		Estimated Solubility Method
logp	1.755		Crippen Method
mcvol	125.370	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
tb	457.10	K	Joback Method
tc	663.91	K	Joback Method
tf	224.74	K	Joback Method
vc	0.477	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.06	J/molxK	457.10	Joback Method
cpg	244.91	J/molxK	491.57	Joback Method
cpg	255.24	J/molxK	526.04	Joback Method
cpg	265.03	J/molxK	560.50	Joback Method
cpg	274.31	J/molxK	594.97	Joback Method
cpg	283.08	J/molxK	629.44	Joback Method
cpg	291.34	J/molxK	663.91	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>h vap:</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>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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