

# Acetic acid, (2-propenylthio)-

<b>Other names:</b>	Acetic acid, (allylthio)- (Allylthio)acetic acid
<b>Inchi:</b>	InChI=1S/C5H8O2S/c1-2-3-8-4-5(6)7/h2H,1,3-4H2,(H,6,7)
<b>InchiKey:</b>	BLSMRHBHPHGMSV-UHFFFAOYSA-N
<b>Formula:</b>	C5H8O2S
<b>SMILES:</b>	C=CCSCC(=O)O
<b>Mol. weight [g/mol]:</b>	132.18
<b>CAS:</b>	20600-63-9

## Physical Properties

Property code	Value	Unit	Source
gf	-153.56	kJ/mol	Joback Method
hf	-244.04	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	56.30	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	0.990		Crippen Method
mcvol	100.800	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
rinpol	1014.00		NIST Webbook
rinpol	1013.00		NIST Webbook
tb	525.31	K	Joback Method
tc	720.69	K	Joback Method
tf	289.50	K	Joback Method
vc	0.376	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.51	J/molxK	525.31	Joback Method
cpg	215.02	J/molxK	557.87	Joback Method
cpg	222.15	J/molxK	590.44	Joback Method
cpg	228.91	J/molxK	623.00	Joback Method
cpg	235.32	J/molxK	655.57	Joback Method

cpg	241.37	J/mol×K	688.13	Joback Method
cpg	247.08	J/mol×K	720.69	Joback Method

## Sources

<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=C20600639&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20600639&amp;Units=SI</a>
<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>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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