Acetic acid, (2-propenylthio)-

Other names:	Acetic acid, (allylthio)-
	(Allylthio)acetic acid
Inchi:	InChI=1S/C5H8O2S/c1-2-3-8-4-5(6)7/h2H,1,3-4H2,(H,6,7)
InchiKey:	BLSMRHBHPHGMSV-UHFFFAOYSA-N
Formula:	C5H8O2S
SMILES:	C=CCSCC(=O)O
Mol. weight [g/mol]:	132.18
CAS:	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/mol×K	525.31	Joback Method
cpg	215.02	J/mol×K	557.87	Joback Method
cpg	222.15	J/mol×K	590.44	Joback Method
cpg	228.91	J/mol×K	623.00	Joback Method
cpg	235.32	J/mol×K	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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20600639&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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