S-1-Propenylmethanethiosulfonate

Other names: 1-Propenyl methanethiosulfonate
Inchi: InChI=1S/C4H8O2S2/c1-3-4-7-8(2,5)6/h3-4H,1-2H3/b4-3+
InchiKey: PGMBAYKBYBXNNR-ONEGZZNKSA-N
Formula: C4H8O2S2
SMILES: CC=CSS(C)(=O)=O
Mol. weight [g/mol]: 152.24

Physical Properties

Property code	Value	Unit	Source
gf	-372.40	kJ/mol	Joback Method
hf	-420.15	kJ/mol	Joback Method
hfus	21.83	kJ/mol	Joback Method
hvap	49.91	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.213		Crippen Method
mcvol	107.360	ml/mol	McGowan Method
pc	5266.25	kPa	Joback Method
rinpol	1179.00		NIST Webbook
tb	411.64	K	Joback Method
tc	609.52	K	Joback Method
tf	202.72	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.07	J/mol×K	411.64	Joback Method
cpg	195.33	J/mol×K	444.62	Joback Method
cpg	204.20	J/mol×K	477.60	Joback Method
cpg	212.67	J/mol×K	510.58	Joback Method
cpg	220.75	J/mol×K	543.56	Joback Method
cpg	228.42	J/mol×K	576.54	Joback Method
cpg	235.70	J/mol×K	609.52	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U322288&Units=SI

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