S-prop-1-en-1-yl propane-1-sulfonothioate

Inchi: InChI=1S/C6H12O2S2/c1-3-5-9-10(7,8)6-4-2/h3,5H,4,6H2,1-2H3/b5-3+
InchiKey: XYAJCUFWPWSDSN-HWKANZROSA-N
Formula: C6H12O2S2
SMILES: CC=CSS(=O)(=O)CCC
Mol. weight [g/mol]: 180.29
CAS: 34139-13-4

Physical Properties

Property code	Value	Unit	Source
gf	-355.56	kJ/mol	Joback Method
hf	-461.43	kJ/mol	Joback Method
hfus	27.01	kJ/mol	Joback Method
hvap	54.36	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	1.993		Crippen Method
mcvol	135.540	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
rinpol	1397.30		NIST Webbook
rinpol	1397.30		NIST Webbook
tb	457.40	K	Joback Method
tc	651.23	K	Joback Method
tf	225.26	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.41	J/mol×K	457.40	Joback Method
cpg	275.28	J/mol×K	489.71	Joback Method
cpg	286.62	J/mol×K	522.01	Joback Method
cpg	297.42	J/mol×K	554.32	Joback Method
cpg	307.70	J/mol×K	586.62	Joback Method
cpg	317.45	J/mol×K	618.93	Joback Method
cpg	326.68	J/mol×K	651.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34139134&Units=SI
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

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