Allyl 1-(methylthio)ethyl disulphide

Inchi: InChI=1S/C6H12S3/c1-4-5-8-9-6(2)7-3/h4,6H,1,5H2,2-3H3
InchiKey: JLUAARRGSDKZGD-UHFFFAOYSA-N
Formula: C6H12S3
SMILES: C=CCSSC(C)SC
Mol. weight [g/mol]: 180.35

Physical Properties

Property code	Value	Unit	Source
gf	184.40	kJ/mol	Joback Method
hf	78.59	kJ/mol	Joback Method
hfus	18.88	kJ/mol	Joback Method
hvap	48.34	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.263		Crippen Method
mcvol	140.150	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
tb	539.26	K	Joback Method
tc	783.98	K	Joback Method
tf	243.82	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.92	J/mol×K	539.26	Joback Method
cpg	295.35	J/mol×K	580.05	Joback Method
cpg	307.04	J/mol×K	620.83	Joback Method
cpg	318.02	J/mol×K	661.62	Joback Method
cpg	328.26	J/mol×K	702.40	Joback Method
cpg	337.77	J/mol×K	743.19	Joback Method
cpg	346.54	J/mol×K	783.98	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=R226025&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