E-1-Chloro-2-methyl-3-propylthio- propene

Inchi: InChI=1S/C6H11ClS/c1-3-4-8-6(2)5-7/h5H,3-4H2,1-2H3/b6-5+
InchiKey: IEONBOZHTJFRFQ-AATRIKPKSA-N
Formula: C6H11ClS
SMILES: CCCSC(C)=CCl
Mol. weight [g/mol]: 150.67

Physical Properties

Property code	Value	Unit	Source
gf	92.50	kJ/mol	Joback Method
hf	-33.61	kJ/mol	Joback Method
hfus	18.52	kJ/mol	Joback Method
hvap	40.19	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.230		Crippen Method
mcvol	119.690	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	832.20		NIST Webbook
rinpol	832.20		NIST Webbook
tb	446.93	K	Joback Method
tc	656.98	K	Joback Method
tf	202.66	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.36	J/mol×K	446.93	Joback Method
cpg	227.25	J/mol×K	481.94	Joback Method
cpg	237.56	J/mol×K	516.95	Joback Method
cpg	247.31	J/mol×K	551.96	Joback Method
cpg	256.52	J/mol×K	586.97	Joback Method
cpg	265.22	J/mol×K	621.97	Joback Method
cpg	273.43	J/mol×K	656.98	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=R153843&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