E-1-(3-Chloro-2-methyl-allylsulfanyl) -butane

Other names: E-1-(3-Chloro-2-methyl-allylthio) -butane
Inchi: InChI=1S/C8H15ClS/c1-3-4-5-10-7-8(2)6-9/h6H,3-5,7H2,1-2H3/b8-6+
InchiKey: LOSAPLMUPWETBL-SOFGYWHQSA-N
Formula: C8H15ClS
SMILES: CCCCSCC(C)=CCl
Mol. weight [g/mol]: 178.72

Physical Properties

Property code	Value	Unit	Source
gf	109.34	kJ/mol	Joback Method
hf	-74.89	kJ/mol	Joback Method
hfus	23.70	kJ/mol	Joback Method
hvap	44.64	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.662		Crippen Method
mcvol	147.870	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1227.60		NIST Webbook
ripol	1587.80		NIST Webbook
tb	492.69	K	Joback Method
tc	697.09	K	Joback Method
tf	225.20	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.71	J/mol×K	492.69	Joback Method
cpg	311.90	J/mol×K	526.76	Joback Method
cpg	324.41	J/mol×K	560.82	Joback Method
cpg	336.25	J/mol×K	594.89	Joback Method
cpg	347.46	J/mol×K	628.96	Joback Method
cpg	358.07	J/mol×K	663.02	Joback Method
cpg	368.09	J/mol×K	697.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R153818&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume