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

Other names: E-1-(3-Chloro-2-methyl-allylthio) -pentane
Inchi: InChI=1S/C9H17ClS/c1-3-4-5-6-11-8-9(2)7-10/h7H,3-6,8H2,1-2H3/b9-7+
InchiKey: IKTZYZGLMACANG-VQHVLOKHSA-N
Formula: C9H17ClS
SMILES: CCCCCSCC(C)=CCl
Mol. weight [g/mol]: 192.75

Physical Properties

Property code	Value	Unit	Source
gf	117.76	kJ/mol	Joback Method
hf	-95.53	kJ/mol	Joback Method
hfus	26.29	kJ/mol	Joback Method
hvap	46.87	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	4.052		Crippen Method
mcvol	161.960	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1331.20		NIST Webbook
rinpol	1331.20		NIST Webbook
ripol	1679.40		NIST Webbook
tb	515.57	K	Joback Method
tc	717.10	K	Joback Method
tf	236.47	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.89	J/mol×K	515.57	Joback Method
cpg	357.03	J/mol×K	549.16	Joback Method
cpg	370.44	J/mol×K	582.75	Joback Method
cpg	383.15	J/mol×K	616.34	Joback Method
cpg	395.18	J/mol×K	649.93	Joback Method
cpg	406.57	J/mol×K	683.51	Joback Method

cpg	417.35	J/mol×K	717.10	Joback Method

Sources

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=R153823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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