Z-1-Chloro-2-methyl-3-propylsulfanyl- propene

Other names: Z-1-Chloro-2-methyl-3-propylthio- propene
Inchi: InChI=1S/C7H13ClS/c1-3-4-9-6-7(2)5-8/h5H,3-4,6H2,1-2H3/b7-5-
InchiKey: CGAZHYSZJPSFJW-ALCCZGGFSA-N
Formula: C7H13ClS
SMILES: CCCSCC(C)=CCl
Mol. weight [g/mol]: 164.70

Physical Properties

Property code	Value	Unit	Source
gf	100.92	kJ/mol	Joback Method
hf	-54.25	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.272		Crippen Method
mcvol	133.780	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	818.80		NIST Webbook
ripol	1166.20		NIST Webbook
tb	469.81	K	Joback Method
tc	677.07	K	Joback Method
tf	213.93	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.50	J/mol×K	469.81	Joback Method
cpg	268.61	J/mol×K	504.35	Joback Method
cpg	280.09	J/mol×K	538.90	Joback Method
cpg	290.95	J/mol×K	573.44	Joback Method
cpg	301.22	J/mol×K	607.98	Joback Method
cpg	310.93	J/mol×K	642.53	Joback Method
cpg	320.10	J/mol×K	677.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R154064&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

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