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

Inchi: InChI=1S/C5H9ClO/c1-5(3-6)4-7-2/h3H,4H2,1-2H3/b5-3-
InchiKey: GAOGDWJPCWMVAG-HYXAFXHYSA-N
Formula: C5H9ClO
SMILES: COCC(C)=CCl
Mol. weight [g/mol]: 120.58

Physical Properties

Property code	Value	Unit	Source
gf	-54.04	kJ/mol	Joback Method
hf	-187.06	kJ/mol	Joback Method
hfus	12.98	kJ/mol	Joback Method
hvap	33.56	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.775		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	812.00		NIST Webbook
rinpol	812.00		NIST Webbook
ripol	1022.90		NIST Webbook
ripol	1022.90		NIST Webbook
tb	377.69	K	Joback Method
tc	563.94	K	Joback Method
tf	179.22	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.95	J/mol×K	377.69	Joback Method
cpg	166.48	J/mol×K	408.73	Joback Method
cpg	174.66	J/mol×K	439.77	Joback Method
cpg	182.50	J/mol×K	470.82	Joback Method
cpg	190.01	J/mol×K	501.86	Joback Method
cpg	197.20	J/mol×K	532.90	Joback Method

cpg	204.08	J/mol×K	563.94	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=R154084&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume