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

Inchi: InChI=1S/C4H7ClO/c1-4(3-5)6-2/h3H,1-2H3/b4-3+
InchiKey: AHLTYTZNLLPVFE-ONEGZZNKSA-N
Formula: C4H7ClO
SMILES: COC(C)=CCl
Mol. weight [g/mol]: 106.55

Physical Properties

Property code	Value	Unit	Source
gf	-62.46	kJ/mol	Joback Method
hf	-166.42	kJ/mol	Joback Method
hfus	10.39	kJ/mol	Joback Method
hvap	31.33	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.733		Crippen Method
mcvol	81.030	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
rinpol	798.80		NIST Webbook
rinpol	798.80		NIST Webbook
ripol	989.50		NIST Webbook
ripol	989.50		NIST Webbook
tb	354.81	K	Joback Method
tc	541.79	K	Joback Method
tf	167.95	K	Joback Method
vc	0.307	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.96	J/mol×K	354.81	Joback Method
cpg	131.92	J/mol×K	385.97	Joback Method
cpg	138.61	J/mol×K	417.14	Joback Method
cpg	145.02	J/mol×K	448.30	Joback Method
cpg	151.18	J/mol×K	479.47	Joback Method
cpg	157.07	J/mol×K	510.63	Joback Method

cpg	162.72	J/mol×K	541.79	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=R153863&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