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

Inchi: InChI=1S/C6H11ClO/c1-3-8-5-6(2)4-7/h4H,3,5H2,1-2H3/b6-4-
InchiKey: GTWUFKWWSZNLSY-XQRVVYSFSA-N
Formula: C6H11ClO
SMILES: CCOCC(C)=CCl
Mol. weight [g/mol]: 134.60

Physical Properties

Property code	Value	Unit	Source
gf	-45.62	kJ/mol	Joback Method
hf	-207.70	kJ/mol	Joback Method
hfus	15.57	kJ/mol	Joback Method
hvap	35.78	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	2.165		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
rinpol	883.20		NIST Webbook
rinpol	883.20		NIST Webbook
ripol	1150.90		NIST Webbook
ripol	1150.90		NIST Webbook
tb	400.57	K	Joback Method
tc	585.74	K	Joback Method
tf	190.49	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.45	J/mol×K	400.57	Joback Method
cpg	203.40	J/mol×K	431.43	Joback Method
cpg	212.94	J/mol×K	462.29	Joback Method
cpg	222.07	J/mol×K	493.15	Joback Method
cpg	230.82	J/mol×K	524.01	Joback Method
cpg	239.19	J/mol×K	554.88	Joback Method

cpg	247.20	J/mol×K	585.74	Joback Method

Sources

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=R154079&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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