3-Hexene, 3-chloro

Inchi: InChI=1S/C6H11Cl/c1-3-5-6(7)4-2/h5H,3-4H2,1-2H3/b6-5-
InchiKey: CRAFRIAAAZWLNA-WAYWQWQTSA-N
Formula: C6H11Cl
SMILES: CCC=C(Cl)CC
Mol. weight [g/mol]: 118.61

Physical Properties

Property code	Value	Unit	Source
gf	59.38	kJ/mol	Joback Method
hf	-75.48	kJ/mol	Joback Method
hfus	14.38	kJ/mol	Joback Method
hvap	33.37	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.929		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	763.00		NIST Webbook
tb	378.15	K	Joback Method
tc	563.28	K	Joback Method
tf	168.26	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.45	J/mol×K	378.15	Joback Method
cpg	181.74	J/mol×K	409.00	Joback Method
cpg	191.53	J/mol×K	439.86	Joback Method
cpg	200.84	J/mol×K	470.71	Joback Method
cpg	209.69	J/mol×K	501.57	Joback Method
cpg	218.09	J/mol×K	532.42	Joback Method
cpg	226.08	J/mol×K	563.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R511229&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume