Heptane, 3-chloro-6-methyl

Inchi: InChI=1S/C8H17Cl/c1-4-8(9)6-5-7(2)3/h7-8H,4-6H2,1-3H3
InchiKey: GMLQONWBBDPDQO-UHFFFAOYSA-N
Formula: C8H17Cl
SMILES: CCC(Cl)CCC(C)C
Mol. weight [g/mol]: 148.67

Physical Properties

Property code	Value	Unit	Source
gf	-0.33	kJ/mol	Joback Method
hf	-234.75	kJ/mol	Joback Method
hfus	13.63	kJ/mol	Joback Method
hvap	37.01	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.440		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	966.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	966.00		NIST Webbook
tb	418.99	K	Joback Method
tc	597.64	K	Joback Method
tf	179.84	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.83	J/mol×K	418.99	Joback Method
cpg	276.35	J/mol×K	448.77	Joback Method
cpg	289.32	J/mol×K	478.54	Joback Method
cpg	301.74	J/mol×K	508.32	Joback Method
cpg	313.63	J/mol×K	538.09	Joback Method
cpg	325.02	J/mol×K	567.87	Joback Method
cpg	335.90	J/mol×K	597.64	Joback Method

dvisc	0.0164704	Pa×s	179.84	Joback Method
dvisc	0.0043901	Pa×s	219.70	Joback Method
dvisc	0.0017563	Pa×s	259.56	Joback Method
dvisc	0.0008967	Pa×s	299.42	Joback Method
dvisc	0.0005362	Pa×s	339.27	Joback Method
dvisc	0.0003572	Pa×s	379.13	Joback Method
dvisc	0.0002571	Pa×s	418.99	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=R116022&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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