

Hexane, 3-chloro-2-methyl

Inchi:	InChI=1S/C7H15Cl/c1-4-5-7(8)6(2)3/h6-7H,4-5H2,1-3H3
InchiKey:	KIXBHIAUACDNJ-UHFFFAOYSA-N
Formula:	C7H15Cl
SMILES:	CCCC(Cl)C(C)C
Mol. weight [g/mol]:	134.65

Physical Properties

Property code	Value	Unit	Source
gf	-8.75	kJ/mol	Joback Method
hf	-214.11	kJ/mol	Joback Method
hfus	11.04	kJ/mol	Joback Method
hvap	34.79	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	3.050		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
tb	396.11	K	Joback Method
tc	575.86	K	Joback Method
tf	168.57	K	Joback Method
vc	0.465	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.12	J/molxK	396.11	Joback Method
cpg	235.48	J/molxK	426.07	Joback Method
cpg	247.33	J/molxK	456.03	Joback Method
cpg	258.70	J/molxK	485.99	Joback Method
cpg	269.58	J/molxK	515.95	Joback Method
cpg	279.99	J/molxK	545.90	Joback Method
cpg	289.96	J/molxK	575.86	Joback Method
dvisc	0.0169478	Paxs	168.57	Joback Method

dvisc	0.0045031	Paxs	206.49	Joback Method
dvisc	0.0018052	Paxs	244.42	Joback Method
dvisc	0.0009251	Paxs	282.34	Joback Method
dvisc	0.0005554	Paxs	320.26	Joback Method
dvisc	0.0003715	Paxs	358.19	Joback Method
dvisc	0.0002684	Paxs	396.11	Joback Method

Sources

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=R116097&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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