

Hexane, 3-chloro-3-methyl-

Other names:	3-Chloro-3-methylhexane
Inchi:	InChI=1S/C7H15Cl/c1-4-6-7(3,8)5-2/h4-6H2,1-3H3
InchiKey:	UTKDCNDVTOWUHW-UHFFFAOYSA-N
Formula:	C7H15Cl
SMILES:	CCCC(C)(Cl)CC
Mol. weight [g/mol]:	134.65
CAS:	43197-78-0

Physical Properties

Property code	Value	Unit	Source
gf	-1.03	kJ/mol	Joback Method
hf	-212.30	kJ/mol	Joback Method
hfus	10.67	kJ/mol	Joback Method
hvap	34.27	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.194		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
tb	393.76	K	Joback Method
tc	576.83	K	Joback Method
tf	200.99	K	Joback Method
vc	0.466	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.71	J/mol×K	393.76	Joback Method
cpg	283.83	J/mol×K	546.32	Joback Method
cpg	273.22	J/mol×K	515.80	Joback Method
cpg	262.03	J/mol×K	485.29	Joback Method
cpg	250.23	J/mol×K	454.78	Joback Method
cpg	237.80	J/mol×K	424.27	Joback Method
cpg	293.88	J/mol×K	576.83	Joback Method
dvisc	0.0003185	Paxs	393.76	Joback Method

dvisc	0.0004349	Paxs	361.63	Joback Method
dvisc	0.0006312	Paxs	329.50	Joback Method
dvisc	0.0009928	Paxs	297.38	Joback Method
dvisc	0.0017428	Paxs	265.25	Joback Method
dvisc	0.0035725	Paxs	233.12	Joback Method
dvisc	0.0092120	Paxs	200.99	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38983e+01
Coeff. B	-3.44222e+03
Coeff. C	-5.46160e+01
Temperature range (K), min.	307.52
Temperature range (K), max.	455.49

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C43197780&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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