Pentane, 3-chloro-2-methyl-

Other names: 3-Chloro-2-methylpentane
Inchi: InChI=1S/C6H13Cl/c1-4-6(7)5(2)3/h5-6H,4H2,1-3H3
InchiKey: FCPXHGJZKRXGJY-UHFFFAOYSA-N
Formula: C6H13Cl
SMILES: CCC(Cl)C(C)C
Mol. weight [g/mol]: 120.62
CAS: 38384-05-3

Physical Properties

Property code	Value	Unit	Source
gf	-17.17	kJ/mol	Joback Method
hf	-193.47	kJ/mol	Joback Method
hfus	8.45	kJ/mol	Joback Method
hvap	32.56	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.660		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	862.00		NIST Webbook
ripol	952.00		NIST Webbook
ripol	956.00		NIST Webbook
ripol	944.00		NIST Webbook
tb	373.23	K	Joback Method
tc	553.82	K	Joback Method
tf	157.30	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.75	J/mol×K	373.23	Joback Method

cpg	236.69	J/mol×K	523.72	Joback Method
cpg	227.35	J/mol×K	493.62	Joback Method
cpg	217.60	J/mol×K	463.52	Joback Method
cpg	207.42	J/mol×K	433.43	Joback Method
cpg	196.81	J/mol×K	403.33	Joback Method
cpg	245.63	J/mol×K	553.82	Joback Method
dvisc	0.0002752	Pa×s	373.23	Joback Method
dvisc	0.0003793	Pa×s	337.24	Joback Method
dvisc	0.0005644	Pa×s	301.25	Joback Method
dvisc	0.0009357	Pa×s	265.26	Joback Method
dvisc	0.0018178	Pa×s	229.28	Joback Method
dvisc	0.0045226	Pa×s	193.29	Joback Method
dvisc	0.0170744	Pa×s	157.30	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42268e+01
Coeff. B	-3.35127e+03
Coeff. C	-4.85000e+01
Temperature range (K), min.	288.92
Temperature range (K), max.	424.40

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=C38384053&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/ci990307l

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
pvap:	Vapor 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