2-Chloro-2,4-dimethylpentane

Inchi: InChI=1S/C7H15Cl/c1-6(2)5-7(3,4)8/h6H,5H2,1-4H3
InchiKey: DQOHPSPKVODKLV-UHFFFAOYSA-N
Formula: C7H15Cl
SMILES: CC(C)CC(C)(C)Cl
Mol. weight [g/mol]: 134.65
CAS: 35951-33-8

Physical Properties

Property code	Value	Unit	Source
gf	-3.47	kJ/mol	Joback Method
hf	-217.58	kJ/mol	Joback Method
hfl	-277.00 ± 2.00	kJ/mol	NIST Webbook
hfus	7.15	kJ/mol	Joback Method
hvap	33.88	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	3.050		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	393.32	K	Joback Method
tc	580.78	K	Joback Method
tf	185.99	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.64	J/mol×K	393.32	Joback Method
cpg	238.14	J/mol×K	424.56	Joback Method
cpg	250.94	J/mol×K	455.81	Joback Method
cpg	263.08	J/mol×K	487.05	Joback Method
cpg	274.56	J/mol×K	518.29	Joback Method
cpg	285.43	J/mol×K	549.54	Joback Method
cpg	295.72	J/mol×K	580.78	Joback Method
dvisc	0.0171872	Pa×s	185.99	Joback Method

dvisc	0.0051996	Pa×s	220.55	Joback Method
dvisc	0.0021747	Pa×s	255.10	Joback Method
dvisc	0.0011198	Pa×s	289.65	Joback Method
dvisc	0.0006643	Pa×s	324.21	Joback Method
dvisc	0.0004358	Pa×s	358.76	Joback Method
dvisc	0.0003078	Pa×s	393.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.33500e+01
Coeff. B	-3.25580e+03
Coeff. C	-5.26700e+01
Temperature range (K), min.	301.92
Temperature range (K), max.	457.70

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35951338&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
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
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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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