Hexane, 1-chloro-5-methyl-

Other names: 1-Chloro-5-methylhexane
Inchi: InChI=1S/C7H15Cl/c1-7(2)5-3-4-6-8/h7H,3-6H2,1-2H3
InchiKey: YESHSLGUAPTMLI-UHFFFAOYSA-N
Formula: C7H15Cl
SMILES: CC(C)CCCCCl
Mol. weight [g/mol]: 134.65
CAS: 33240-56-1

Physical Properties

Property code	Value	Unit	Source
gf	-6.31	kJ/mol	Joback Method
hf	-208.83	kJ/mol	Joback Method
hfus	14.56	kJ/mol	Joback Method
hvap	35.17	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	3.051		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
tb	396.55	K	Joback Method
tc	572.19	K	Joback Method
tf	183.57	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.17	J/mol×K	396.55	Joback Method
cpg	235.16	J/mol×K	425.82	Joback Method
cpg	246.67	J/mol×K	455.10	Joback Method
cpg	257.72	J/mol×K	484.37	Joback Method
cpg	268.31	J/mol×K	513.64	Joback Method
cpg	278.47	J/mol×K	542.91	Joback Method
cpg	288.19	J/mol×K	572.19	Joback Method
dvisc	0.0087444	Pa×s	183.57	Joback Method

dvisc	0.0030894	Pa×s	219.07	Joback Method
dvisc	0.0014589	Pa×s	254.56	Joback Method
dvisc	0.0008278	Pa×s	290.06	Joback Method
dvisc	0.0005315	Pa×s	325.56	Joback Method
dvisc	0.0003723	Pa×s	361.05	Joback Method
dvisc	0.0002780	Pa×s	396.55	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52290e+01
Coeff. B	-3.88859e+03
Coeff. C	-5.90640e+01
Temperature range (K), min.	319.32
Temperature range (K), max.	451.16

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=C33240561&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume