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: ---

Physical Properties

Property code	Value	Unit	Source
af	0.3860		Cheméo Relay (1.0)
gf	-6.31	kJ/mol	Joback Method
hf	-235.78	kJ/mol	Cheméo Relay (1.0)
hfus	14.56	kJ/mol	Joback Method
hvap	44.28	kJ/mol	Cheméo Relay (1.0)
ie	10.30	eV	Cheméo Relay (1.0)
log10ws	-3.97		Cheméo Relay (1.0)
logp	3.051		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
tb	419.01	K	Cheméo Relay (1.0)
tc	604.54	K	Cheméo Relay (1.0)
tf	190.15	K	Cheméo Relay (1.0)
vc	0.444	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33240561&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

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
ie:	Ionization energy
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