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
af	0.3088		Cheméo Relay (1.0)
gf	-1.03	kJ/mol	Joback Method
hf	-233.31	kJ/mol	Cheméo Relay (1.0)
hfus	10.67	kJ/mol	Joback Method
hvap	40.59	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.57		Cheméo Relay (1.0)
logp	3.194		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
tb	395.77	K	Cheméo Relay (1.0)
tc	595.80	K	Cheméo Relay (1.0)
tf	179.16	K	Cheméo Relay (1.0)
vc	0.440	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.71	J/mol×K	393.76	Joback Method
cpg	237.80	J/mol×K	424.27	Joback Method
cpg	250.23	J/mol×K	454.78	Joback Method
cpg	262.03	J/mol×K	485.29	Joback Method
cpg	273.22	J/mol×K	515.80	Joback Method
cpg	283.83	J/mol×K	546.32	Joback Method
cpg	293.88	J/mol×K	576.83	Joback Method
dvisc	0.0092120	Pa×s	200.99	Joback Method

dvisc	0.0035725	Pa×s	233.12	Joback Method
dvisc	0.0017428	Pa×s	265.25	Joback Method
dvisc	0.0009928	Pa×s	297.38	Joback Method
dvisc	0.0006312	Pa×s	329.50	Joback Method
dvisc	0.0004349	Pa×s	361.63	Joback Method
dvisc	0.0003185	Pa×s	393.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

Cheméo Relay (1.0):

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=C43197780&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

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
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