Heptane, 3-chloro-3-methyl-

Other names: 3-Chloro-3-methylheptane
Inchi: InChI=1S/C8H17Cl/c1-4-6-7-8(3,9)5-2/h4-7H2,1-3H3
InchiKey: XGAHNVWATDXDPG-UHFFFAOYSA-N
Formula: C8H17Cl
SMILES: CCCCC(C)(Cl)CC
Mol. weight [g/mol]: 148.67
CAS: 5272-02-6

Physical Properties

Property code	Value	Unit	Source
gf	7.39	kJ/mol	Joback Method
hf	-232.94	kJ/mol	Joback Method
hfus	13.26	kJ/mol	Joback Method
hvap	36.49	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.584		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
tb	416.64	K	Joback Method
tc	598.52	K	Joback Method
tf	212.26	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.68	J/mol×K	416.64	Joback Method
cpg	328.78	J/mol×K	568.20	Joback Method
cpg	317.26	J/mol×K	537.89	Joback Method
cpg	305.11	J/mol×K	507.58	Joback Method
cpg	292.32	J/mol×K	477.27	Joback Method
cpg	278.85	J/mol×K	446.95	Joback Method
cpg	339.71	J/mol×K	598.52	Joback Method
dvisc	0.0002979	Pa×s	416.64	Joback Method

dvisc	0.0004084	Pa×s	382.58	Joback Method
dvisc	0.0005954	Pa×s	348.51	Joback Method
dvisc	0.0009419	Pa×s	314.45	Joback Method
dvisc	0.0016656	Pa×s	280.39	Joback Method
dvisc	0.0034485	Pa×s	246.32	Joback Method
dvisc	0.0090186	Pa×s	212.26	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39315e+01
Coeff. B	-3.62925e+03
Coeff. C	-6.21220e+01
Temperature range (K), min.	328.12
Temperature range (K), max.	483.15

Sources

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=C5272026&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

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