3-Chloroheptane

Other names: Heptane, 3-chloro-
Inchi: InChI=1S/C7H15Cl/c1-3-5-6-7(8)4-2/h7H,3-6H2,1-2H3
InchiKey: DMKNOEJJJSHSML-UHFFFAOYSA-N
Formula: C7H15Cl
SMILES: CCCCC(Cl)CC
Mol. weight [g/mol]: 134.65
CAS: 999-52-0

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	-3.02		Crippen Method
logp	3.194		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	960.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	906.00		NIST Webbook
ripol	1057.00		NIST Webbook
ripol	1078.00		NIST Webbook
ripol	1076.00		NIST Webbook
ripol	1076.00		NIST Webbook
ripol	1057.00		NIST Webbook
ripol	1069.00		NIST Webbook
ripol	1074.00		NIST Webbook
ripol	1057.00		NIST Webbook
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

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=C999520&Units=SI
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume