1,7-Dichloroheptane

Other names: 1,7-Dichloro-n-heptane
Heptane, 1,7-dichloro-
Inchi: InChI=1S/C7H14Cl2/c8-6-4-2-1-3-5-7-9/h1-7H2
InchiKey: PSEMXLIZFGUOGC-UHFFFAOYSA-N
Formula: C7H14Cl2
SMILES: ClCCCCCCCCl
Mol. weight [g/mol]: 169.09
CAS: 821-76-1

Physical Properties

Property code	Value	Unit	Source
gf	-15.80	kJ/mol	Joback Method
hf	-219.29	kJ/mol	Joback Method
hfus	22.28	kJ/mol	Joback Method
hvap	61.20	kJ/mol	NIST Webbook
log10ws	-3.06		Crippen Method
logp	3.414		Crippen Method
mcvol	133.970	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
tb	434.42	K	Joback Method
tc	613.21	K	Joback Method
tf	228.49	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.95	J/mol×K	613.21	Joback Method
cpg	302.92	J/mol×K	583.41	Joback Method
cpg	293.46	J/mol×K	553.61	Joback Method
cpg	283.56	J/mol×K	523.82	Joback Method
cpg	273.20	J/mol×K	494.02	Joback Method
cpg	262.38	J/mol×K	464.22	Joback Method
cpg	251.07	J/mol×K	434.42	Joback Method

dvisc	0.0047500	Pa×s	228.49	Joback Method
dvisc	0.0003122	Pa×s	434.42	Joback Method
dvisc	0.0004045	Pa×s	400.10	Joback Method
dvisc	0.0005503	Pa×s	365.78	Joback Method
dvisc	0.0007978	Pa×s	331.46	Joback Method
dvisc	0.0012604	Pa×s	297.13	Joback Method
dvisc	0.0022437	Pa×s	262.81	Joback Method
hvapt	52.30	kJ/mol	448.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	397.70	K	4.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48712e+01
Coeff. B	-4.11519e+03
Coeff. C	-7.07400e+01
Temperature range (K), min.	352.92
Temperature range (K), max.	501.21

Sources

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

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=C821761&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume