1,2-dichloroheptane

Inchi: InChI=1S/C7H14Cl2/c1-2-3-4-5-7(9)6-8/h7H,2-6H2,1H3
InchiKey: WBCSJABQCRFUCP-UHFFFAOYSA-N
Formula: C7H14Cl2
SMILES: CCCCCC(Cl)CCl
Mol. weight [g/mol]: 169.09
CAS: 10575-87-8

Physical Properties

Property code	Value	Unit	Source
gf	-18.24	kJ/mol	Joback Method
hf	-224.57	kJ/mol	Joback Method
hfus	18.76	kJ/mol	Joback Method
hvap	53.20	kJ/mol	NIST Webbook
log10ws	-3.17		Crippen Method
logp	3.413		Crippen Method
mcvol	133.970	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
ripol	1366.00		NIST Webbook
ripol	1366.00		NIST Webbook
tb	433.98	K	Joback Method
tc	616.82	K	Joback Method
tf	213.49	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.14	J/mol×K	433.98	Joback Method
cpg	262.79	J/mol×K	464.45	Joback Method
cpg	273.93	J/mol×K	494.93	Joback Method
cpg	284.57	J/mol×K	525.40	Joback Method
cpg	294.73	J/mol×K	555.87	Joback Method
cpg	304.42	J/mol×K	586.35	Joback Method
cpg	313.66	J/mol×K	616.82	Joback Method

dvisc	0.0074245	Pa×s	213.49	Joback Method
dvisc	0.0029334	Pa×s	250.24	Joback Method
dvisc	0.0014701	Pa×s	286.99	Joback Method
dvisc	0.0008619	Pa×s	323.74	Joback Method
dvisc	0.0005634	Pa×s	360.48	Joback Method
dvisc	0.0003984	Pa×s	397.23	Joback Method
dvisc	0.0002988	Pa×s	433.98	Joback Method
hvapt	49.00	kJ/mol	409.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44465e+01
Coeff. B	-3.95841e+03
Coeff. C	-6.93500e+01
Temperature range (K), min.	348.92
Temperature range (K), max.	502.67

Sources

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=C10575878&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume