2,4-dichlorohexane

Inchi: InChI=1S/C6H12Cl2/c1-3-6(8)4-5(2)7/h5-6H,3-4H2,1-2H3
InchiKey: LHEKJUGTNGWYIA-UHFFFAOYSA-N
Formula: C6H12Cl2
SMILES: CCC(Cl)CC(C)Cl
Mol. weight [g/mol]: 155.06
CAS: ---

Physical Properties

Property code	Value	Unit	Source
gf	-29.10	kJ/mol	Joback Method
hf	-209.21	kJ/mol	Joback Method
hfus	12.64	kJ/mol	Joback Method
hvap	36.94	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	3.021		Crippen Method
mcvol	119.880	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
ripol	1276.00		NIST Webbook
ripol	1244.00		NIST Webbook
tb	410.66	K	Joback Method
tc	599.28	K	Joback Method
tf	187.22	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.29	J/mol×K	410.66	Joback Method
cpg	223.08	J/mol×K	442.10	Joback Method
cpg	233.37	J/mol×K	473.53	Joback Method
cpg	243.19	J/mol×K	504.97	Joback Method
cpg	252.55	J/mol×K	536.41	Joback Method
cpg	261.47	J/mol×K	567.84	Joback Method
cpg	269.95	J/mol×K	599.28	Joback Method

dvisc	0.0130601	Pa×s	187.22	Joback Method
dvisc	0.0041501	Pa×s	224.46	Joback Method
dvisc	0.0018276	Pa×s	261.70	Joback Method
dvisc	0.0009873	Pa×s	298.94	Joback Method
dvisc	0.0006113	Pa×s	336.18	Joback Method
dvisc	0.0004165	Pa×s	373.42	Joback Method
dvisc	0.0003042	Pa×s	410.66	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50501e+01
Coeff. B	-4.00000e+03
Coeff. C	-6.47630e+01
Temperature range (K), min.	335.72
Temperature range (K), max.	475.50

Sources

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=R211820&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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