

1,4-Dichlorohexane

Other names:	Hexane, 1,4-dichloro
Inchi:	InChI=1S/C6H12Cl2/c1-2-6(8)4-3-5-7/h6H,2-5H2,1H3
InchiKey:	QUBRHRAWRVZUFZ-UHFFFAOYSA-N
Formula:	C6H12Cl2
SMILES:	CCC(Cl)CCCCI
Mol. weight [g/mol]:	155.06
CAS:	50635-35-3

Physical Properties

Property code	Value	Unit	Source
gf	-26.66	kJ/mol	Joback Method
hf	-203.93	kJ/mol	Joback Method
hfus	16.17	kJ/mol	Joback Method
hvap	37.33	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	3.023		Crippen Method
mcvol	119.880	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1058.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1058.00		NIST Webbook
ripol	1419.00		NIST Webbook
tb	411.10	K	Joback Method
tc	595.37	K	Joback Method
tf	202.22	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.27	J/molxK	411.10	Joback Method
cpg	222.72	J/molxK	441.81	Joback Method
cpg	232.70	J/molxK	472.52	Joback Method
cpg	242.24	J/molxK	503.23	Joback Method

cpg	251.35	J/mol×K	533.95	Joback Method
cpg	260.04	J/mol×K	564.66	Joback Method
cpg	268.32	J/mol×K	595.37	Joback Method
dvisc	0.0074186	Paxs	202.22	Joback Method
dvisc	0.0029798	Paxs	237.03	Joback Method
dvisc	0.0015119	Paxs	271.85	Joback Method
dvisc	0.0008949	Paxs	306.66	Joback Method
dvisc	0.0005894	Paxs	341.47	Joback Method
dvisc	0.0004194	Paxs	376.29	Joback Method
dvisc	0.0003162	Paxs	411.10	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.69346e+01
Coeff. B	-4.66271e+03
Coeff. C	-6.96280e+01
Temperature range (K), min.	349.72
Temperature range (K), max.	470.78

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50635353&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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