Cyclohexane, 1,1-dichloro-

Other names: 1,1-Dichlorocyclohexane
Inchi: InChI=1S/C6H10Cl2/c7-6(8)4-2-1-3-5-6/h1-5H2
InchiKey: LQRDJCBZCLUBRY-UHFFFAOYSA-N
Formula: C6H10Cl2
SMILES: ClC1(Cl)CCCCC1
Mol. weight [g/mol]: 153.05
CAS: 2108-92-1

Physical Properties

Property code	Value	Unit	Source
gf	-5.26	kJ/mol	Joback Method
hf	-129.09	kJ/mol	Joback Method
hfus	5.23	kJ/mol	Joback Method
hvap	37.00	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.124		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
rinpol	978.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	981.00		NIST Webbook
tb	431.33	K	Joback Method
tc	662.65	K	Joback Method
tf	248.50	K	Joback Method
tt	236.59 ± 0.10	K	NIST Webbook
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.47	J/mol×K	431.33	Joback Method
cpg	206.89	J/mol×K	469.88	Joback Method
cpg	220.08	J/mol×K	508.44	Joback Method
cpg	232.18	J/mol×K	546.99	Joback Method
cpg	243.32	J/mol×K	585.55	Joback Method
cpg	253.62	J/mol×K	624.10	Joback Method
cpg	263.23	J/mol×K	662.65	Joback Method
hfust	1.47	kJ/mol	236.00	NIST Webbook
hvapt	43.50	kJ/mol	389.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.25730e+01
Coeff. B	-3.00555e+03
Coeff. C	-7.68170e+01
Temperature range (K), min.	321.46
Temperature range (K), max.	490.72

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=C2108921&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume