

1,6-Dichlorocyclohexene

Inchi:	InChI=1S/C6H8Cl2/c7-5-3-1-2-4-6(5)8/h3,6H,1-2,4H2
InchiKey:	YDCVSMGKDQZJSD-UHFFFAOYSA-N
Formula:	C6H8Cl2
SMILES:	C1C=CCCC1Cl
Mol. weight [g/mol]:	151.03

Physical Properties

Property code	Value	Unit	Source
gf	20.56	kJ/mol	Joback Method
hf	-98.02	kJ/mol	Joback Method
hfus	12.36	kJ/mol	Joback Method
hvap	39.10	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.900		Crippen Method
mvol	104.720	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
rinpol	1067.00		NIST Webbook
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tb	435.23	K	Joback Method
tc	660.08	K	Joback Method
tf	237.88	K	Joback Method
vc	0.389	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.47	J/molxK	435.23	Joback Method
cpg	190.55	J/molxK	472.71	Joback Method
cpg	201.94	J/molxK	510.18	Joback Method
cpg	212.65	J/molxK	547.66	Joback Method
cpg	222.70	J/molxK	585.13	Joback Method
cpg	232.12	J/molxK	622.61	Joback Method
cpg	240.91	J/molxK	660.08	Joback Method
dvisc	0.0032773	Paxs	237.88	Joback Method

dvisc	0.0017801	Paxs	270.77	Joback Method
dvisc	0.0011035	Paxs	303.66	Joback Method
dvisc	0.0007511	Paxs	336.56	Joback Method
dvisc	0.0005475	Paxs	369.45	Joback Method
dvisc	0.0004203	Paxs	402.34	Joback Method
dvisc	0.0003358	Paxs	435.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R591681&Units=SI
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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