1,3-Dichlorocyclohexene

Inchi: InChI=1S/C6H8Cl2/c7-5-2-1-3-6(8)4-5/h4-5H,1-3H2
InchiKey: XQROSXTWWDQLMZ-UHFFFAOYSA-N
Formula: C6H8Cl2
SMILES: ClC1=CC(Cl)CCC1
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
mcvol	104.720	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
rinpol	1088.00		NIST Webbook
tb	435.23	K	Joback Method
tc	660.08	K	Joback Method
tf	237.88	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.47	J/mol×K	435.23	Joback Method
cpg	190.55	J/mol×K	472.71	Joback Method
cpg	201.94	J/mol×K	510.18	Joback Method
cpg	212.65	J/mol×K	547.66	Joback Method
cpg	222.70	J/mol×K	585.13	Joback Method
cpg	232.12	J/mol×K	622.61	Joback Method
cpg	240.91	J/mol×K	660.08	Joback Method
dvisc	0.0032773	Pa×s	237.88	Joback Method
dvisc	0.0017801	Pa×s	270.77	Joback Method

dvisc	0.0011035	Pa×s	303.66	Joback Method
dvisc	0.0007511	Pa×s	336.56	Joback Method
dvisc	0.0005475	Pa×s	369.45	Joback Method
dvisc	0.0004203	Pa×s	402.34	Joback Method
dvisc	0.0003358	Pa×s	435.23	Joback Method

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=R591676&Units=SI

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