

Cyclohexene, 3-chloro-

Other names:	3-Cyclohexenyl chloride 3-Chloro-1-cyclohexene 3-Chlorocyclohexene 3-Chlorocyclohexene-1
Inchi:	InChI=1S/C6H9Cl/c7-6-4-2-1-3-5-6/h2,4,6H,1,3,5H2
InchiKey:	LNGQLHZIYFQUIR-UHFFFAOYSA-N
Formula:	C6H9Cl
SMILES:	C1C1C=CCCC1
Mol. weight [g/mol]:	116.59
CAS:	2441-97-6

Physical Properties

Property code	Value	Unit	Source
gf	42.12	kJ/mol	Joback Method
hf	-70.81	kJ/mol	Joback Method
hfus	8.55	kJ/mol	Joback Method
hvap	34.06	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.334		Crippen Method
mcvol	92.480	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
rinpol	857.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	857.00		NIST Webbook
ripol	1215.00		NIST Webbook
ripol	1215.00		NIST Webbook
tb	392.82	K	Joback Method
tc	608.17	K	Joback Method
tf	195.44	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	151.19	J/mol×K	392.82	Joback Method
cpg	210.00	J/mol×K	572.28	Joback Method
cpg	199.61	J/mol×K	536.39	Joback Method
cpg	188.56	J/mol×K	500.49	Joback Method
cpg	176.82	J/mol×K	464.60	Joback Method
cpg	164.37	J/mol×K	428.71	Joback Method
cpg	219.75	J/mol×K	608.17	Joback Method
dvisc	0.0003137	Pa×s	392.82	Joback Method
dvisc	0.0004029	Pa×s	359.92	Joback Method
dvisc	0.0005441	Pa×s	327.03	Joback Method
dvisc	0.0007859	Pa×s	294.13	Joback Method
dvisc	0.0012453	Pa×s	261.23	Joback Method
dvisc	0.0022533	Pa×s	228.34	Joback Method
dvisc	0.0049779	Pa×s	195.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2441976&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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