

2-Chlorocyclohexanol

Other names:	Cyclohexanol, 2-chloro-
Inchi:	InChI=1S/C6H11ClO/c7-5-3-1-2-4-6(5)8/h5-6,8H,1-4H2
InchiKey:	NYEWDMNNOXFGDX-UHFFFAOYSA-N
Formula:	C6H11ClO
SMILES:	OC1CCCCC1Cl
Mol. weight [g/mol]:	134.60
CAS:	1561-86-0

Physical Properties

Property code	Value	Unit	Source
gf	-132.37	kJ/mol	Joback Method
hf	-301.16	kJ/mol	Joback Method
hfus	12.49	kJ/mol	Joback Method
hvap	50.13	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.529		Crippen Method
mcvol	102.650	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
rinpol	1032.10		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1017.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1659.00		NIST Webbook
ripol	1658.00		NIST Webbook
tb	481.17	K	Joback Method
tc	681.95	K	Joback Method
tf	251.26	K	Joback Method
vc	0.371	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	216.66	J/molxK	481.17	Joback Method
cpg	229.30	J/molxK	514.63	Joback Method
cpg	241.30	J/molxK	548.10	Joback Method
cpg	252.67	J/molxK	581.56	Joback Method
cpg	263.43	J/molxK	615.02	Joback Method
cpg	273.59	J/molxK	648.48	Joback Method
cpg	283.17	J/molxK	681.95	Joback Method
dvisc	0.0353626	Paxs	251.26	Joback Method
dvisc	0.0087916	Paxs	289.58	Joback Method
dvisc	0.0030260	Paxs	327.90	Joback Method
dvisc	0.0013020	Paxs	366.22	Joback Method
dvisc	0.0006572	Paxs	404.53	Joback Method
dvisc	0.0003734	Paxs	442.85	Joback Method
dvisc	0.0002322	Paxs	481.17	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1561860&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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

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