

Cyclohexane, 1,2,3,4,5,6-hexachloro-

Other names:	1,2,3,4,5,6-Hexachlorocyclohexane HCH BHC Benzene hexachloride Compound-666 ENT 8,601 Hexachlor Hexachlorocyclohexane Hexaklor Latka 666 Benzene hexachloride (BHC) BHC or HCH
Inchi:	InChI=1S/C6H6Cl6/c7-1-2(8)4(10)6(12)5(11)3(1)9/h1-6H
InchiKey:	JLYXXMFPNIAWKQ-UHFFFAOYSA-N
Formula:	C6H6Cl6
SMILES:	<chem>C1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl</chem>
Mol. weight [g/mol]:	290.83
CAS:	608-73-1

Physical Properties

Property code	Value	Unit	Source
gf	-86.04	kJ/mol	Joback Method
hf	-308.99	kJ/mol	Joback Method
hfus	33.67	kJ/mol	Joback Method
hvap	54.14	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.644		Crippen Method
mcpvol	157.980	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1792.00		NIST Webbook
rinpol	1778.00		NIST Webbook
ripol	2452.00		NIST Webbook
ripol	2452.00		NIST Webbook
ripol	2452.00		NIST Webbook
tb	557.46	K	Joback Method
tc	799.93	K	Joback Method
tf	323.08	K	Joback Method

vc	0.594	m ³ /kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.54	J/mol×K	557.46	Joback Method
cpg	314.57	J/mol×K	597.87	Joback Method
cpg	326.75	J/mol×K	638.28	Joback Method
cpg	338.08	J/mol×K	678.70	Joback Method
cpg	348.54	J/mol×K	719.11	Joback Method
cpg	358.13	J/mol×K	759.52	Joback Method
cpg	366.85	J/mol×K	799.93	Joback Method
dvisc	0.0015575	Pa×s	323.08	Joback Method
dvisc	0.0011967	Pa×s	362.14	Joback Method
dvisc	0.0009679	Pa×s	401.21	Joback Method
dvisc	0.0008129	Pa×s	440.27	Joback Method
dvisc	0.0007025	Pa×s	479.33	Joback Method
dvisc	0.0006205	Pa×s	518.40	Joback Method
dvisc	0.0005577	Pa×s	557.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C608731&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
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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