

1-Hexanol, 6-chloro-

Other names:	1-Chloro-6-hydroxyhexane 6-Chloro-1-hexanol 6-Chlorohexanol Hexamethylene chlorohydrin 1-Chloro-6-hexanol 6-chlorohexan-1-ol
Inchi:	InChI=1S/C6H13ClO/c7-5-3-1-2-4-6-8/h8H,1-6H2
InchiKey:	JNTPTNCGDAGEJ-UHFFFAOYSA-N
Formula:	C6H13ClO
SMILES:	OCCCCCCI
Mol. weight [g/mol]:	136.62
CAS:	2009-83-8

Physical Properties

Property code	Value	Unit	Source
gf	-149.11	kJ/mol	Joback Method
hf	-335.14	kJ/mol	Joback Method
hfus	19.58	kJ/mol	Joback Method
hvap	50.01	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.778		Crippen Method
mcvol	113.510	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
tb	466.29	K	Joback Method
tc	633.66	K	Joback Method
tf	248.12	K	Joback Method
vc	0.440	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.37	J/mol×K	466.29	Joback Method
cpg	275.80	J/mol×K	605.77	Joback Method
cpg	268.01	J/mol×K	577.87	Joback Method

cpg	259.88	J/molxK	549.98	Joback Method
cpg	251.40	J/molxK	522.08	Joback Method
cpg	242.57	J/molxK	494.19	Joback Method
cpg	283.26	J/molxK	633.66	Joback Method
dvisc	0.0002210	Paxs	466.29	Joback Method
dvisc	0.0003651	Paxs	429.93	Joback Method
dvisc	0.0006615	Paxs	393.57	Joback Method
dvisc	0.0013530	Paxs	357.20	Joback Method
dvisc	0.0032543	Paxs	320.84	Joback Method
dvisc	0.0097963	Paxs	284.48	Joback Method
dvisc	0.0407336	Paxs	248.12	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.20	K	1.90	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2009838&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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