

1-Chloro-4-methylcyclohexane

Inchi:	InChI=1S/C7H13Cl/c1-6-2-4-7(8)5-3-6/h6-7H,2-5H2,1H3
InchiKey:	KNEUJTFLMQRIFD-UHFFFAOYSA-N
Formula:	C7H13Cl
SMILES:	CC1CCC(Cl)CC1
Mol. weight [g/mol]:	132.63
CAS:	931-68-0

Physical Properties

Property code	Value	Unit	Source
gf	12.87	kJ/mol	Joback Method
hf	-169.57	kJ/mol	Joback Method
hfus	10.99	kJ/mol	Joback Method
hvap	35.68	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.804		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
tb	411.87	K	Joback Method
tc	622.19	K	Joback Method
tf	201.71	K	Joback Method
vc	0.408	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.40	J/mol×K	411.87	Joback Method
cpg	276.29	J/mol×K	587.14	Joback Method
cpg	263.21	J/mol×K	552.09	Joback Method
cpg	249.40	J/mol×K	517.03	Joback Method
cpg	234.84	J/mol×K	481.98	Joback Method
cpg	219.51	J/mol×K	446.92	Joback Method
cpg	288.64	J/mol×K	622.19	Joback Method
dvisc	0.0003137	Paxs	411.87	Joback Method
dvisc	0.0003947	Paxs	376.84	Joback Method

dvisc	0.0005205	Paxs	341.82	Joback Method
dvisc	0.0007311	Paxs	306.79	Joback Method
dvisc	0.0011211	Paxs	271.76	Joback Method
dvisc	0.0019507	Paxs	236.74	Joback Method
dvisc	0.0041145	Paxs	201.71	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C931680&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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