Cyclohexanone, 2-chloro-

Other names: «alpha»-Chlorocyclohexanone
2-Chlorocyclohexanone
Inchi: InChI=1S/C6H9ClO/c7-5-3-1-2-4-6(5)8/h5H,1-4H2
InchiKey: CCHNWURRBFGQCD-UHFFFAOYSA-N
Formula: C6H9ClO
SMILES: O=C1CCCCC1Cl
Mol. weight [g/mol]: 132.59
CAS: 822-87-7

Physical Properties

Property code	Value	Unit	Source
gf	-110.43	kJ/mol	Joback Method
hf	-266.29	kJ/mol	Joback Method
hfus	6.84	kJ/mol	Joback Method
hvap	38.01	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.737		Crippen Method
mcvol	98.350	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
rinpol	1026.00		NIST Webbook
tb	461.48	K	Joback Method
tc	695.41	K	Joback Method
tf	262.90	K	Joback Method
vc	0.360	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.33	J/mol×K	461.48	Joback Method
cpg	204.24	J/mol×K	500.47	Joback Method
cpg	217.50	J/mol×K	539.46	Joback Method
cpg	230.12	J/mol×K	578.44	Joback Method
cpg	242.06	J/mol×K	617.43	Joback Method
cpg	253.33	J/mol×K	656.42	Joback Method

cpg	263.90	J/mol×K	695.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.70	K	1.30	NIST Webbook
tbrp	367.00 ± 2.00	K	2.10	NIST Webbook

Sources

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=C822877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume