

3-Chloro-5,5-dimethylcyclohex-2-enone

Other names:	3-Chloro-5,5-dimethyl-2-cyclohexen-1-one 5,5-Dimethyl-3-chloro-2-cyclohexen-1-one 3-Chloro-5,5-dimethyl-2-cyclohexenone 5,5-Dimethyl-3-chlorocyclohex-2-enone
Inchi:	InChI=1S/C8H11ClO/c1-8(2)4-6(9)3-7(10)5-8/h3H,4-5H2,1-2H3
InchiKey:	PJYTYJGMJDIKEJ-UHFFFAOYSA-N
Formula:	C8H11ClO
SMILES:	CC1(C)CC(=O)C=C(Cl)C1
Mol. weight [g/mol]:	158.62
CAS:	17530-69-7

Physical Properties

Property code	Value	Unit	Source
affp	867.90	kJ/mol	NIST Webbook
basg	836.00	kJ/mol	NIST Webbook
gf	-78.75	kJ/mol	Joback Method
hf	-246.02	kJ/mol	Joback Method
hfus	6.55	kJ/mol	Joback Method
hvap	42.27	kJ/mol	Joback Method
ie	9.35	eV	NIST Webbook
log10ws	-2.61		Crippen Method
logp	2.498		Crippen Method
mcvol	122.230	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	511.62	K	Joback Method
tc	751.42	K	Joback Method
tf	322.62	K	Joback Method
vc	0.457	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.16	J/mol×K	511.62	Joback Method
cpg	273.55	J/mol×K	551.59	Joback Method

cpg	287.04	J/mol×K	591.55	Joback Method
cpg	299.74	J/mol×K	631.52	Joback Method
cpg	311.75	J/mol×K	671.49	Joback Method
cpg	323.17	J/mol×K	711.46	Joback Method
cpg	334.11	J/mol×K	751.42	Joback Method

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=C17530697&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
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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