

# Cyclohexanone, oxime

<b>Other names:</b>	(Hydroxyimino)cyclohexane Antioxidant D NSC 6300 cyclohexanone oxime
<b>Inchi:</b>	InChI=1S/C6H11NO/c8-7-6-4-2-1-3-5-6/h8H,1-5H2
<b>InchiKey:</b>	VEZUQRBDRNJBRY-UHFFFAOYSA-N
<b>Formula:</b>	C6H11NO
<b>SMILES:</b>	ON=C1CCCCC1
<b>Mol. weight [g/mol]:</b>	113.16
<b>CAS:</b>	100-64-1

## Physical Properties

Property code	Value	Unit	Source
chs	-3779.90 ± 2.30	kJ/mol	NIST Webbook
chs	-3723.00 ± 4.20	kJ/mol	NIST Webbook
hf	-74.88	kJ/mol	NIST Webbook
hfs	-153.20 ± 2.50	kJ/mol	NIST Webbook
hfus	12.45	kJ/mol	Thermodynamics of Cyclohexanone Oxime
hsub	79.00 ± 2.00	kJ/mol	NIST Webbook
hsub	78.32 ± 0.30	kJ/mol	NIST Webbook
hvap	63.10 ± 1.00	kJ/mol	NIST Webbook
ie	8.97 ± 0.03	eV	NIST Webbook
log10ws	-1.05		Crippen Method
logp	1.781		Crippen Method
mcvol	96.090	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
rinpol	1074.00		NIST Webbook
rinpol	1074.00		NIST Webbook
ss	185.08	J/mol×K	NIST Webbook
ss	185.12	J/mol×K	NIST Webbook
tb	481.20	K	NIST Webbook
tc	744.08	K	Joback Method
tf	362.00 ± 4.00	K	NIST Webbook
tt	362.50 ± 0.30	K	NIST Webbook
tt	362.50 ± 0.50	K	NIST Webbook

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	199.38	J/mol×K	298.15	NIST Webbook
cps	199.34	J/mol×K	298.15	NIST Webbook
hfust	12.45	kJ/mol	362.20	NIST Webbook
hfust	12.70	kJ/mol	362.50	NIST Webbook
hfust	12.70	kJ/mol	362.60	NIST Webbook
hsubt	79.90 ± 0.70	kJ/mol	318.00	NIST Webbook
hsubt	76.50 ± 1.00	kJ/mol	378.00	NIST Webbook
hsubt	74.00 ± 0.30	kJ/mol	354.00	NIST Webbook
hvapt	58.66	kJ/mol	367.80	NIST Webbook
hvapt	58.70 ± 0.60	kJ/mol	368.00	NIST Webbook
hvapt	59.50 ± 0.50	kJ/mol	408.50	NIST Webbook

## Sources

**Solid-Liquid Equilibrium and Activity Coefficients for Binary Mixtures of Caprolactam + Cyclohexanone Oxime with Room-Temperature Ionic Liquids:**

<https://www.doi.org/10.1021/je1005054>

<https://www.doi.org/10.1021/je700546r>

[https://en.wikipedia.org/wiki/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=C100641&Units=SI>

**Solid-Liquid Equilibrium and Activity Coefficients for Caprolactam + Cinnamyl-3-methylimidazolium**

<https://www.doi.org/10.1021/je7000683>

**Bis(trifluoromethylsulfonyl)imide and Cyclohexanone Oxime + Thermodynamic Properties of Mixtures Containing Ionic Liquid Cation: ammomethinium, tetraethyl ammonium, bis(trifluoromethylsulfonyl)imide, guanidinium sulfate, USHG-1 gas liquid chromatography and cyclohexanone method:** methyl tert-butyl ether system:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

<https://www.doi.org/10.1021/je0602723>

<https://www.doi.org/10.1016/j.fluid.2016.03.002>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

**chs:** Standard solid enthalpy of combustion

**cps:** Solid phase heat capacity

**hf:** Enthalpy of formation at standard conditions

**hfs:** Solid phase enthalpy of formation at standard conditions

<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ss:</b>	Solid phase molar entropy at standard conditions
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature

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