Cyclohexanone, oxime

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

Physical Properties

Property code	Value	Unit	Source
chs	-3723.00 ± 4.20	kJ/mol	NIST Webbook
chs	-3779.90 ± 2.30	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	78.32 ± 0.30	kJ/mol	NIST Webbook
hsub	79.00 ± 2.00	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 ± 0.50	K	NIST Webbook
tt	362.50 ± 0.30	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	76.50 ± 1.00	kJ/mol	378.00	NIST Webbook
hsubt	74.00 ± 0.30	kJ/mol	354.00	NIST Webbook
hsubt	79.90 ± 0.70	kJ/mol	318.00	NIST Webbook
hvapt	59.50 ± 0.50	kJ/mol	408.50	NIST Webbook
hvapt	58.66	kJ/mol	367.80	NIST Webbook
hvapt	58.70 ± 0.60	kJ/mol	368.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Solid-Liquid Equilibrium and Activity Coefficients for Caprolactam + 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide and Cyclohexanone Oxime + 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide: https://www.doi.org/10.1021/je7000683

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100641&Units=SI

Determination and modeling for solid-liquid phase equilibrium of ternary caprolactam + cyclohexanone oxime + methyl tert-butyl ether system: https://www.doi.org/10.1016/j.fluid.2016.03.002

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Experimental Study of Thermodynamic Properties of Mixtures Containing Ionic Liquid 1-Ethyl-3-methylimidazolium Ethyl Sulfate Using Gas-Liquid Chromatography and Transpiration Method: https://www.doi.org/10.1021/je0602723

Solid-Liquid Equilibrium and Activity Coefficients for Binary Mixtures of Cyclohexanone Oxime with Room-Temperature Ionic Liquids : https://www.doi.org/10.1021/je1005054

Thermodynamics of Cyclohexanone Oxime: https://www.doi.org/10.1021/je700546r

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

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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