

# 3-Ethoxy-2-cyclohexen-1-one

<b>Other names:</b>	3-Ethoxy-2-cyclohexene-1-one 3-Ethoxy-2-cyclohexenone 2-Cyclohexen-1-one, 3-ethoxy- 3-ethoxycyclohex-2-ene-1-one
<b>Inchi:</b>	InChI=1S/C8H12O2/c1-2-10-8-5-3-4-7(9)6-8/h6H,2-5H2,1H3
<b>InchiKey:</b>	JWCFJPLIRVYENQ-UHFFFAOYSA-N
<b>Formula:</b>	C8H12O2
<b>SMILES:</b>	CCOC1=CC(=O)CCC1
<b>Mol. weight [g/mol]:</b>	140.18
<b>CAS:</b>	5323-87-5

## Physical Properties

Property code	Value	Unit	Source
gf	-158.62	kJ/mol	Joback Method
hf	-357.40	kJ/mol	Joback Method
hfus	8.77	kJ/mol	Joback Method
hvap	41.75	kJ/mol	Joback Method
ie	8.69 ± 0.05	eV	NIST Webbook
log10ws	-1.78		Crippen Method
logp	1.660		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
tb	501.04	K	Joback Method
tc	722.96	K	Joback Method
tf	295.27	K	Joback Method
vc	0.428	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.61	J/mol×K	501.04	Joback Method
cpg	269.18	J/mol×K	538.03	Joback Method
cpg	283.15	J/mol×K	575.01	Joback Method
cpg	296.49	J/mol×K	612.00	Joback Method

cpg	309.19	J/mol×K	648.98	Joback Method
cpg	321.22	J/mol×K	685.97	Joback Method
cpg	332.57	J/mol×K	722.96	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.20	K	0.10	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5323875&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5323875&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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