

# 2-Ethyl-3-methoxy-2-cyclopentenone

<b>Inchi:</b>	InChI=1S/C8H12O2/c1-3-6-7(9)4-5-8(6)10-2/h3-5H2,1-2H3
<b>InchiKey:</b>	CGBUGQQOHMWSAF-UHFFFAOYSA-N
<b>Formula:</b>	C8H12O2
<b>SMILES:</b>	CCC1=C(OC)CCC1=O
<b>Mol. weight [g/mol]:</b>	140.18
<b>CAS:</b>	25112-86-1

## Physical Properties

Property code	Value	Unit	Source
gf	-156.15	kJ/mol	Joback Method
hf	-362.71	kJ/mol	Joback Method
hfus	10.48	kJ/mol	Joback Method
hvap	42.24	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.660		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
tb	501.75	K	Joback Method
tc	716.67	K	Joback Method
tf	311.31	K	Joback Method
vc	0.436	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.12	J/molxK	501.75	Joback Method
cpg	268.35	J/molxK	537.57	Joback Method
cpg	281.10	J/molxK	573.39	Joback Method
cpg	293.33	J/molxK	609.21	Joback Method
cpg	305.04	J/molxK	645.03	Joback Method
cpg	316.20	J/molxK	680.85	Joback Method
cpg	326.80	J/molxK	716.67	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C25112861&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25112861&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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