

# Cyclohexanone, 4-ethyl-

<b>Other names:</b>	4-Ethylcyclohexanone
<b>Inchi:</b>	InChI=1S/C8H14O/c1-2-7-3-5-8(9)6-4-7/h7H,2-6H2,1H3
<b>InchiKey:</b>	OKSDJGWHKXFVME-UHFFFAOYSA-N
<b>Formula:</b>	C8H14O
<b>SMILES:</b>	CCC1CCC(=O)CC1
<b>Mol. weight [g/mol]:</b>	126.20
<b>CAS:</b>	5441-51-0

## Physical Properties

Property code	Value	Unit	Source
gf	-81.66	kJ/mol	Joback Method
hf	-291.83	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	38.08	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.156		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	466.20	K	NIST Webbook
tc	690.17	K	Joback Method
tf	255.52	K	Joback Method
vc	0.423	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.75	J/mol×K	469.81	Joback Method
cpg	263.69	J/mol×K	506.54	Joback Method
cpg	279.88	J/mol×K	543.26	Joback Method
cpg	295.31	J/mol×K	579.99	Joback Method
cpg	309.98	J/mol×K	616.71	Joback Method
cpg	323.89	J/mol×K	653.44	Joback Method
cpg	337.02	J/mol×K	690.17	Joback Method

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44791e+01
Coeff. B	-3.89955e+03
Coeff. C	-7.07400e+01
Temperature range (K), min.	345.52
Temperature range (K), max.	496.10

## Sources

<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5441510&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5441510&amp;Units=SI</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>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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