

# 2-Cyclohepten-1-one

<b>Other names:</b>	Tropilene 2-Cycloheptenone cyclohept-2-en-1-one
<b>Inchi:</b>	InChI=1S/C7H10O/c8-7-5-3-1-2-4-6-7/h3,5H,1-2,4,6H2
<b>InchiKey:</b>	WZCRDVTWUYLPTR-UHFFFAOYSA-N
<b>Formula:</b>	C7H10O
<b>SMILES:</b>	O=C1C=CCCCC1
<b>Mol. weight [g/mol]:</b>	110.15
<b>CAS:</b>	1121-66-0

## Physical Properties

Property code	Value	Unit	Source
gf	-64.51	kJ/mol	Joback Method
hf	-199.23	kJ/mol	Joback Method
hfus	3.28	kJ/mol	Joback Method
hvap	36.62	kJ/mol	Joback Method
ie	9.25	eV	NIST Webbook
log10ws	-1.78		Crippen Method
logp	1.686		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	1020.00		NIST Webbook
rinpol	1024.00		NIST Webbook
tb	455.03	K	Joback Method
tc	690.86	K	Joback Method
tf	245.73	K	Joback Method
vc	0.346	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.47	J/mol×K	455.03	Joback Method
cpg	202.54	J/mol×K	494.34	Joback Method
cpg	216.89	J/mol×K	533.64	Joback Method

cpg	230.50	J/mol×K	572.95	Joback Method
cpg	243.38	J/mol×K	612.25	Joback Method
cpg	255.51	J/mol×K	651.56	Joback Method
cpg	266.87	J/mol×K	690.86	Joback Method

## Sources

<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=C1121660&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121660&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>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>rinpola:</b>	Non-polar retention indices
<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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