

# 1H-Inden-1-one, octahydro-

<b>Other names:</b>	1-Indanone, hexahydro- 1-Hydrindanone Bicyclo[4.3.0]nonan-7-one
<b>Inchi:</b>	InChI=1S/C9H14O/c10-9-6-5-7-3-1-2-4-8(7)9/h7-8H,1-6H2
<b>InchiKey:</b>	ATKSQUYIHKMKTG-UHFFFAOYSA-N
<b>Formula:</b>	C9H14O
<b>SMILES:</b>	O=C1CCC2CCCCC12
<b>Mol. weight [g/mol]:</b>	138.21
<b>CAS:</b>	29927-85-3

## Physical Properties

Property code	Value	Unit	Source
gf	-12.49	kJ/mol	Joback Method
hf	-239.67	kJ/mol	Joback Method
hfus	8.55	kJ/mol	Joback Method
hvap	40.22	kJ/mol	Joback Method
ie	9.08 ± 0.08	eV	NIST Webbook
log10ws	-2.18		Crippen Method
logp	2.156		Crippen Method
mcvol	117.520	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	499.43	K	Joback Method
tc	734.32	K	Joback Method
tf	284.73	K	Joback Method
vc	0.436	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.47	J/molxK	499.43	Joback Method
cpg	296.85	J/molxK	538.58	Joback Method
cpg	315.07	J/molxK	577.73	Joback Method
cpg	332.18	J/molxK	616.87	Joback Method
cpg	348.20	J/molxK	656.02	Joback Method

cpg	363.18	J/mol×K	695.17	Joback Method
cpg	377.14	J/mol×K	734.32	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=C29927853&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C29927853&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>hvac:</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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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