

# 2H-Inden-2-one, octahydro-3a-methyl-, cis-

<b>Other names:</b>	2-Indanone, hexahydro-3a-methyl-, cis- 3a-Methyloctahydro-2H-inden-2-one, (Z)-
<b>Inchi:</b>	InChI=1S/C10H16O/c1-10-5-3-2-4-8(10)6-9(11)7-10/h8H,2-7H2,1H3/t8-,10+/m0/s1
<b>InchiKey:</b>	AMBOSHXMUMOHBF-WCBMZHEXSA-N
<b>Formula:</b>	C10H16O
<b>SMILES:</b>	CC12CCCCC1CC(=O)C2
<b>Mol. weight [g/mol]:</b>	152.23
<b>CAS:</b>	13351-29-6

## Physical Properties

Property code	Value	Unit	Source
chs	-5873.80 ± 3.40	kJ/mol	NIST Webbook
gf	-9.56	kJ/mol	Joback Method
hf	-287.00 ± 3.40	kJ/mol	NIST Webbook
hfs	-347.90 ± 3.40	kJ/mol	NIST Webbook
hfus	4.84	kJ/mol	Joback Method
hsub	60.92 ± 0.17	kJ/mol	NIST Webbook
hsub	60.90 ± 0.20	kJ/mol	NIST Webbook
hvap	41.29	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.546		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
tb	522.55	K	Joback Method
tc	763.29	K	Joback Method
tf	319.90	K	Joback Method
vc	0.490	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.27	J/mol×K	522.55	Joback Method
cpg	344.37	J/mol×K	562.67	Joback Method
cpg	363.07	J/mol×K	602.80	Joback Method

cpg	380.54	J/mol×K	642.92	Joback Method
cpg	396.93	J/mol×K	683.04	Joback Method
cpg	412.39	J/mol×K	723.17	Joback Method
cpg	427.09	J/mol×K	763.29	Joback Method

## Sources

<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=C13351296&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13351296&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>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<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>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hsub:</b>	Enthalpy of sublimation 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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