

# (3a«alpha»,4«alpha»,7«alpha»,7a«alpha»)-3a,4,7,7

<b>Other names:</b>	endo-3a,4,7,7a-Tetrahydro-4,7-methanoinden-1-one endo-Dicyclopentadienone
<b>Inchi:</b>	InChI=1S/C10H10O/c11-9-4-3-8-6-1-2-7(5-6)10(8)9/h1-4,6-8,10H,5H2
<b>InchiKey:</b>	USCIQHADNYEBHX-UHFFFAOYSA-N
<b>Formula:</b>	C10H10O
<b>SMILES:</b>	O=C1C=CC2C3C=CC(C3)C12
<b>Mol. weight [g/mol]:</b>	146.19
<b>CAS:</b>	5530-96-1

## Physical Properties

Property code	Value	Unit	Source
chs	-5348.37	kJ/mol	NIST Webbook
gf	133.09	kJ/mol	Joback Method
hf	-79.97	kJ/mol	Joback Method
hfs	-15.90	kJ/mol	NIST Webbook
hfus	16.99	kJ/mol	Joback Method
hvap	42.29	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.564		Crippen Method
mvol	112.150	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	514.16	K	Joback Method
tc	750.16	K	Joback Method
tf	318.26	K	Joback Method
vc	0.436	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.38	J/molxK	514.16	Joback Method
cpg	292.43	J/molxK	553.49	Joback Method
cpg	308.23	J/molxK	592.83	Joback Method
cpg	322.86	J/molxK	632.16	Joback Method
cpg	336.42	J/molxK	671.49	Joback Method

cpg	348.98	J/mol×K	710.83	Joback Method
cpg	360.64	J/mol×K	750.16	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=C5530961&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5530961&amp;Units=SI</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>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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