

# 3H-Cyclopenta[a]pentalen-3-one-1,2,3a,5,6,6a,7,7a

<b>Inchi:</b>	InChI=1S/C14H20O/c1-13(2)7-9-6-10-4-5-12(15)14(10,3)11(9)8-13/h8-10H,4-7H2,1-3H3
<b>InchiKey:</b>	BYIJYWQTZCVKLX-BFVZDQMLSA-N
<b>Formula:</b>	C14H20O
<b>SMILES:</b>	CC1(C)C=C2C(CC3CCC(=O)C23C)C1
<b>Mol. weight [g/mol]:</b>	204.31

## Physical Properties

Property code	Value	Unit	Source
gf	104.10	kJ/mol	Joback Method
hf	-207.46	kJ/mol	Joback Method
hfus	11.04	kJ/mol	Joback Method
hvap	49.43	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.348		Crippen Method
mcvol	172.810	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpola	1446.00		NIST Webbook
rinpola	1446.00		NIST Webbook
tb	616.25	K	Joback Method
tc	859.92	K	Joback Method
tf	419.38	K	Joback Method
vc	0.662	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.67	J/molxK	616.25	Joback Method
cpg	509.45	J/molxK	656.86	Joback Method
cpg	529.04	J/molxK	697.47	Joback Method
cpg	547.77	J/molxK	738.09	Joback Method
cpg	565.98	J/molxK	778.70	Joback Method
cpg	583.99	J/molxK	819.31	Joback Method
cpg	602.15	J/molxK	859.92	Joback Method

# Sources

<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=R404963&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R404963&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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