

# Ethanone, 1-(2,3-dihydro-1,1,2,3,3,6-hexamethyl-1H-inden-5-yl)

<b>Other names:</b>	Ketone, 1,1,2,3,3,6-hexamethyl-5-indanyl methyl Phantolid Phantolide 5-Acetyl-1,1,2,3,3,6-hexamethylindan 6-Acetyl-1,1,2,3,3,5-hexamethylindan 1,1,2,3,3,6-hexamethylindan-5-yl methyl ketone
<b>Inchi:</b>	InChI=1S/C17H24O/c1-10-8-14-15(9-13(10)11(2)18)17(6,7)12(3)16(14,4)5/h8-9,12H,1-7
<b>InchiKey:</b>	VDBHOHJWUDKDRW-UHFFFAOYSA-N
<b>Formula:</b>	C17H24O
<b>SMILES:</b>	CC(=O)c1cc2c(cc1C)C(C)(C)C(C)C2(C)C
<b>Mol. weight [g/mol]:</b>	244.37
<b>CAS:</b>	15323-35-0

## Physical Properties

Property code	Value	Unit	Source
gf	81.21	kJ/mol	Joback Method
hf	-242.07	kJ/mol	Joback Method
hfus	21.94	kJ/mol	Joback Method
hvap	61.44	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.403		Crippen Method
mcvol	217.340	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
tb	681.73	K	Joback Method
tc	904.75	K	Joback Method
tf	336.60	K	NIST Webbook
vc	0.837	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.83	J/mol×K	681.73	Joback Method
cpg	625.71	J/mol×K	718.90	Joback Method
cpg	643.98	J/mol×K	756.07	Joback Method

cpg	661.87	J/mol×K	793.24	Joback Method
cpg	679.63	J/mol×K	830.41	Joback Method
cpg	697.48	J/mol×K	867.58	Joback Method
cpg	715.66	J/mol×K	904.75	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.00	K	0.30	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C15323350&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15323350&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.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>

## 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>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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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