

# Ethanone, 1-[2,3-dihydro-1,1,2,6-tetramethyl-3-(1-methylethyl)

Other names:

Traseolide

1-[2,3-dihydro-1,1,2,6-tetramethyl-3-(1-methylethyl)-1H-inden-5-yl]ethan-1-one

Inchi:

InChI=1S/C18H26O/c1-10(2)17-12(4)18(6,7)16-8-11(3)14(13(5)19)9-15(16)17/h8-10,12,

InchiKey:

IMRYETFJNLKUHK-UHFFFAOYSA-N

Formula:

C18H26O

SMILES:

CC(=O)c1cc2c(cc1C)C(C)(C)C(C)C2C(C)C

Mol. weight [g/mol]:

258.40

CAS:

68140-48-7

## Physical Properties

Property code	Value	Unit	Source
gf	92.68	kJ/mol	Joback Method
hf	-283.23	kJ/mol	Joback Method
hfus	27.31	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.865		Crippen Method
mvol	231.430	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
tb	703.93	K	Joback Method
tc	919.95	K	Joback Method
tf	424.89	K	Joback Method
vc	0.888	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.55	J/mol×K	703.93	Joback Method
cpg	686.14	J/mol×K	739.93	Joback Method
cpg	704.87	J/mol×K	775.94	Joback Method
cpg	722.86	J/mol×K	811.94	Joback Method
cpg	740.26	J/mol×K	847.94	Joback Method
cpg	757.19	J/mol×K	883.94	Joback Method
cpg	773.80	J/mol×K	919.95	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C68140487&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C68140487&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>
<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>hvp:</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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