

# 5,7-Octadien-4-one, 2,6-dimethyl-, (Z)-

<b>Other names:</b>	cis-Tagetone Tagetone (Z) (Z)-5,7-Octadien-4-one, 3,6-dimethyl (Z)-Tagetone (Z)-2,6-Dimethylocta-5,7-dien-4-one trans-Tagetone (5E)-2,6-Dimethyl-5,7-octadien-4-one (E)-Tagetone (E)-2,6-Dimethylocta-5,7-dien-4-one
<b>Inchi:</b>	InChI=1S/C10H16O/c1-5-9(4)7-10(11)6-8(2)3/h5,7-8H,1,6H2,2-4H3/b9-7-
<b>InchiKey:</b>	RJXKHBTYHGBOKV-CLFYSBASSA-N
<b>Formula:</b>	C10H16O
<b>SMILES:</b>	<chem>C=CC(C)=CC(=O)CC(C)C</chem>
<b>Mol. weight [g/mol]:</b>	152.23
<b>CAS:</b>	3588-18-9

## Physical Properties

Property code	Value	Unit	Source
gf	61.47	kJ/mol	Joback Method
hf	-134.73	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	43.58	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.734		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1153.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1138.00		NIST Webbook

rinpol	1155.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1122.00	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1132.00	NIST Webbook
rinpol	1132.00	NIST Webbook
rinpol	1120.00	NIST Webbook
rinpol	1122.00	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1120.00	NIST Webbook
rinpol	1146.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1146.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1151.00	NIST Webbook
rinpol	1126.00	NIST Webbook
rinpol	1129.00	NIST Webbook
rinpol	1146.00	NIST Webbook
rinpol	1122.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1135.00	NIST Webbook
rinpol	1125.00	NIST Webbook
rinpol	1156.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1159.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1122.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1155.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1156.00	NIST Webbook
ripol	1459.00	NIST Webbook
ripol	1501.00	NIST Webbook
ripol	1522.00	NIST Webbook
ripol	1517.00	NIST Webbook
ripol	1500.00	NIST Webbook

ripol	1459.00		NIST Webbook
ripol	1500.00		NIST Webbook
tb	482.35	K	Joback Method
tc	674.03	K	Joback Method
tf	216.59	K	Joback Method
vc	0.557	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.71	J/mol×K	482.35	Joback Method
cpg	321.86	J/mol×K	514.30	Joback Method
cpg	335.28	J/mol×K	546.24	Joback Method
cpg	347.99	J/mol×K	578.19	Joback Method
cpg	360.04	J/mol×K	610.14	Joback Method
cpg	371.44	J/mol×K	642.09	Joback Method
cpg	382.25	J/mol×K	674.03	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=C3588189&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3588189&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>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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	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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