

# trans-«beta»-Ocimene

<b>Other names:</b>	1,3,6-Octatriene, 3,7-dimethyl-, (E)- «beta»-trans-Ocimene trans-3,7-Dimethyl-1,3,6-Octatriene Ocimene, trans-«beta»- (E)-Ocimene trans-Ocimene (3E)-3,7-Dimethyl-1,3,6-octatriene «beta»-(E)-Ocimene «beta»-Ocimene, (E)- (E)- «beta»-Ocimene (E)-3,7-Dimethyl-1,3,6-octatriene Ocimene, trans t-«beta»-Ocimene Ocimene trans-beta-form (E)-3,7-Dimethylocta-1,3,6-triene t-Ocimene «beta»-Ocymene, (E)- ocimene-x (E)- «beta»-Ocimene (trans-ocimene) (E)-«beta»-3,7-dimethyl-1,3,6-octatriene ((E)-«beta»-ocimene) (E)- «beta»-Ocymene
<b>Inchi:</b>	InChI=1S/C10H16/c1-5-10(4)8-6-7-9(2)3/h5,7-8H,1,6H2,2-4H3/b10-8+
<b>InchiKey:</b>	IHPKGUQCSIINRJ-CSKARUKUSA-N
<b>Formula:</b>	C10H16
<b>SMILES:</b>	<chem>C=CC(C)=CCC=C(C)C</chem>
<b>Mol. weight [g/mol]:</b>	136.23
<b>CAS:</b>	3779-61-1

## Physical Properties

Property code	Value	Unit	Source
gf	264.50	kJ/mol	Joback Method
hf	90.56	kJ/mol	Joback Method
hfus	18.16	kJ/mol	Joback Method
hvap	37.26	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.475		Crippen Method

mcvol	138.860	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	1050.00		NIST Webbook
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ripol	1241.70		NIST Webbook
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tb	432.96	K	Joback Method
tc	622.27	K	Joback Method
tf	162.62	K	Joback Method
vc	0.538	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.68	J/mol×K	432.96	Joback Method
cpg	283.41	J/mol×K	464.51	Joback Method
cpg	297.33	J/mol×K	496.06	Joback Method
cpg	310.50	J/mol×K	527.62	Joback Method
cpg	322.94	J/mol×K	559.17	Joback Method
cpg	334.71	J/mol×K	590.72	Joback Method
cpg	345.84	J/mol×K	622.27	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=C3779611&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3779611&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>

# 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>h vap:</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>m cvol:</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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