

# (Z)-«beta»-Ocimenol

<b>Inchi:</b>	InChI=1S/C10H16O/c1-5-9(4)7-10(11)6-8(2)3/h5-7,10-11H,1H2,2-4H3/b9-7-
<b>InchiKey:</b>	DUCHBDMNWUYHGL-CLFYBASSA-N
<b>Formula:</b>	C10H16O
<b>SMILES:</b>	C=CC(C)=CC(O)C=C(C)C
<b>Mol. weight [g/mol]:</b>	152.23

## Physical Properties

Property code	Value	Unit	Source
gf	125.24	kJ/mol	Joback Method
hf	-66.95	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.446		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinsol	1165.00		NIST Webbook
tb	524.70	K	Joback Method
tc	708.61	K	Joback Method
tf	208.44	K	Joback Method
vc	0.551	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.95	J/mol×K	524.70	Joback Method
cpg	338.47	J/mol×K	555.35	Joback Method
cpg	350.31	J/mol×K	586.00	Joback Method
cpg	361.52	J/mol×K	616.65	Joback Method
cpg	372.13	J/mol×K	647.31	Joback Method
cpg	382.18	J/mol×K	677.96	Joback Method
cpg	391.71	J/mol×K	708.61	Joback Method

# Sources

<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>
<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=R617293&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R617293&amp;Units=SI</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>r inpol:</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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