

# occidenol

<b>Inchi:</b>	InChI=1S/C15H24O2/c1-11-10-17-8-7-15(4)6-5-12(9-13(11)15)14(2,3)16/h7-8,10,12-13,
<b>InchiKey:</b>	MHBHVBZBPFDCSL-UHFFFAOYSA-N
<b>Formula:</b>	C15H24O2
<b>SMILES:</b>	CC1=COC=CC2(C)CCC(C(C)(C)O)CC12
<b>Mol. weight [g/mol]:</b>	236.35
<b>CAS:</b>	27548-56-7

## Physical Properties

Property code	Value	Unit	Source
gf	-46.59	kJ/mol	Joback Method
hf	-432.12	kJ/mol	Joback Method
hfus	21.86	kJ/mol	Joback Method
hvap	69.35	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.628		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1674.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1669.00		NIST Webbook
ripol	2328.00		NIST Webbook
ripol	2328.00		NIST Webbook
tb	692.20	K	Joback Method
tc	910.60	K	Joback Method
tf	400.60	K	Joback Method
vc	0.748	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.40	J/mol×K	692.20	Joback Method
cpg	630.31	J/mol×K	728.60	Joback Method
cpg	648.19	J/mol×K	765.00	Joback Method

cpg	665.20	J/mol×K	801.40	Joback Method
cpg	681.50	J/mol×K	837.80	Joback Method
cpg	697.24	J/mol×K	874.20	Joback Method
cpg	712.58	J/mol×K	910.60	Joback Method

## Sources

<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=C27548567&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C27548567&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>

## 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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