

# Aromadendrene oxide

<b>Inchi:</b>	InChI=1S/C15H24O/c1-9-4-5-10-12(9)13-11(14(13,2)3)6-7-15(10)8-16-15/h9-13H,4-8H2
<b>InchiKey:</b>	XPGWKKLDFXNBPJ-HVRXJVPLSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	CC1CCC2C1C1C(CCC23CO3)C1(C)C
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	186.09	kJ/mol	Joback Method
hf	-230.43	kJ/mol	Joback Method
hfus	23.64	kJ/mol	Joback Method
hvap	50.09	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.484		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	1662.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
tb	587.25	K	Joback Method
tc	815.53	K	Joback Method
tf	388.70	K	Joback Method
vc	0.710	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.52	J/molxK	587.25	Joback Method
cpg	568.21	J/molxK	625.30	Joback Method
cpg	590.27	J/molxK	663.34	Joback Method
cpg	611.03	J/molxK	701.39	Joback Method
cpg	630.84	J/molxK	739.44	Joback Method
cpg	650.04	J/molxK	777.48	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R604698&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R604698&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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>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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