

# Oxo-agarospirol

<b>Inchi:</b>	InChI=1S/C15H24O2/c1-11-5-4-6-13(10-16)15(11)8-7-12(9-15)14(2,3)17/h6,10-12,17H,4
<b>InchiKey:</b>	OKBGEROEGQDLFK-KKXIITGPSA-N
<b>Formula:</b>	C15H24O2
<b>SMILES:</b>	CC1CCC=C(C=O)C12CCC(C(C)(C)O)C2
<b>Mol. weight [g/mol]:</b>	236.35

## Physical Properties

Property code	Value	Unit	Source
gf	-77.85	kJ/mol	Joback Method
hf	-437.32	kJ/mol	Joback Method
hfus	17.04	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.099		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1823.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1822.00		NIST Webbook
tb	710.48	K	Joback Method
tc	924.83	K	Joback Method
tf	418.79	K	Joback Method
vc	0.765	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.32	J/molxK	710.48	Joback Method
cpg	639.30	J/molxK	746.20	Joback Method
cpg	656.38	J/molxK	781.93	Joback Method
cpg	672.72	J/molxK	817.65	Joback Method
cpg	688.47	J/molxK	853.38	Joback Method
cpg	703.80	J/molxK	889.10	Joback Method
cpg	718.85	J/molxK	924.83	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=R613053&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R613053&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>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>rinpola:</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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