

# «beta»-Agarofuran

<b>Inchi:</b>	InChI=1S/C15H24O/c1-11-6-5-8-14(4)9-7-12-10-15(11,14)16-13(12,2)3/h12H,1,5-10H2,2
<b>InchiKey:</b>	XWTXUKLVEPDOQT-SNPRPXQ TSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	<chem>C=C1CCCC2(C)CCC3CC12OC3(C)C</chem>
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	164.15	kJ/mol	Joback Method
hf	-175.39	kJ/mol	Joback Method
hfus	11.71	kJ/mol	Joback Method
hvap	50.15	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.080		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinpola	1473.00		NIST Webbook
rinpola	1473.00		NIST Webbook
rinpola	1474.00		NIST Webbook
rinpola	1474.00		NIST Webbook
tb	597.79	K	Joback Method
tc	836.76	K	Joback Method
tf	409.78	K	Joback Method
vc	0.721	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.39	J/molxK	597.79	Joback Method
cpg	558.80	J/molxK	637.62	Joback Method
cpg	579.78	J/molxK	677.45	Joback Method
cpg	599.81	J/molxK	717.28	Joback Method
cpg	619.32	J/molxK	757.11	Joback Method
cpg	638.78	J/molxK	796.94	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=R612901&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R612901&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>

## 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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