

# helifolen-12-al (syn-anti-anti)

<b>Inchi:</b>	InChI=1S/C15H22O/c1-11-4-5-12-14(3,10-16)13(2)6-8-15(11,12)9-7-13/h6,8,10-12H,4-5
<b>InchiKey:</b>	IVGPPCYQIKEJMO-UHFFFAOYSA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	CC1CCC2C13C=CC(C)(CC3)C2(C)C=O
<b>Mol. weight [g/mol]:</b>	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	132.02	kJ/mol	Joback Method
hf	-169.61	kJ/mol	Joback Method
hfus	11.57	kJ/mol	Joback Method
hvap	52.01	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpola	1578.00		NIST Webbook
rinpola	1578.00		NIST Webbook
tb	610.56	K	Joback Method
tc	846.37	K	Joback Method
tf	411.57	K	Joback Method
vc	0.726	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.43	J/mol×K	610.56	Joback Method
cpg	549.02	J/mol×K	649.86	Joback Method
cpg	568.38	J/mol×K	689.16	Joback Method
cpg	586.96	J/mol×K	728.46	Joback Method
cpg	605.21	J/mol×K	767.77	Joback Method
cpg	623.58	J/mol×K	807.07	Joback Method
cpg	642.54	J/mol×K	846.37	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R233657&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R233657&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.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>

# 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>hvp:</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>rinp:</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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