

# Helifolen-12-oic acid (syn-anti-anti), methyl ester

Inchi:	InChI=1S/C16H24O2/c1-11-5-6-12-15(3,13(17)18-4)14(2)7-9-16(11,12)10-8-14/h7,9,11-
InchiKey:	BGRIBZWMDPIJFU-UHFFFAOYSA-N
Formula:	C16H24O2
SMILES:	COC(=O)C1(C)C2CCC(C)C23C=CC1(C)CC3
Mol. weight [g/mol]:	248.36

## Physical Properties

Property code	Value	Unit	Source
gf	6.04	kJ/mol	Joback Method
hf	-349.47	kJ/mol	Joback Method
hfus	14.66	kJ/mol	Joback Method
hvap	56.67	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.568		Crippen Method
mcvol	206.860	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1662.00		NIST Webbook
rinpol	1662.00		NIST Webbook
ripol	2060.00		NIST Webbook
tb	661.07	K	Joback Method
tc	893.85	K	Joback Method
tf	453.00	K	Joback Method
vc	0.788	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.03	J/molxK	661.07	Joback Method
cpg	630.94	J/molxK	699.87	Joback Method
cpg	651.10	J/molxK	738.66	Joback Method
cpg	670.92	J/molxK	777.46	Joback Method
cpg	690.83	J/molxK	816.26	Joback Method
cpg	711.25	J/molxK	855.05	Joback Method
cpg	732.59	J/molxK	893.85	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R503090&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R503090&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>

# 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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</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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