

# Helifolen-12-oic acid (syn,syn,syn)

<b>Inchi:</b>	InChI=1S/C15H22O2/c1-10-4-5-11-14(3,12(16)17)13(2)6-8-15(10,11)9-7-13/h6,8,10-11H
<b>InchiKey:</b>	CFOAFRDJZWKHED-UHFFFAOYSA-N
<b>Formula:</b>	C15H22O2
<b>SMILES:</b>	CC1CCC2C13C=CC(C)(CC3)C2(C)C(=O)O
<b>Mol. weight [g/mol]:</b>	234.33

## Physical Properties

Property code	Value	Unit	Source
gf	-34.20	kJ/mol	Joback Method
hf	-348.84	kJ/mol	Joback Method
hfus	14.97	kJ/mol	Joback Method
hvap	68.71	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.480		Crippen Method
mvol	192.770	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rmpol	1780.00		NIST Webbook
rmpol	1780.00		NIST Webbook
tb	707.95	K	Joback Method
tc	929.41	K	Joback Method
tf	480.32	K	Joback Method
vc	0.734	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.53	J/mol×K	707.95	Joback Method
cpg	610.11	J/mol×K	744.86	Joback Method
cpg	627.53	J/mol×K	781.77	Joback Method
cpg	645.18	J/mol×K	818.68	Joback Method
cpg	663.42	J/mol×K	855.59	Joback Method
cpg	682.63	J/mol×K	892.50	Joback Method
cpg	703.20	J/mol×K	929.41	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=R503194&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R503194&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>

# 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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