

# Filifolide A

<b>Inchi:</b>	InChI=1S/C10H14O2/c1-6-5-10(2,3)7-4-8(6)12-9(7)11/h5,7-8H,4H2,1-3H3
<b>InchiKey:</b>	JHKNAYGQYUKKDQ-UHFFFAOYSA-N
<b>Formula:</b>	C10H14O2
<b>SMILES:</b>	CC1=CC(C)(C)C2CC1OC2=O
<b>Mol. weight [g/mol]:</b>	166.22

## Physical Properties

Property code	Value	Unit	Source
gf	-70.96	kJ/mol	Joback Method
hf	-344.94	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	46.28	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.904		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
ripol	1996.00		NIST Webbook
tb	544.70	K	Joback Method
tc	777.48	K	Joback Method
tf	359.03	K	Joback Method
vc	0.504	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.26	J/mol×K	544.70	Joback Method
cpg	355.17	J/mol×K	583.50	Joback Method
cpg	371.01	J/mol×K	622.29	Joback Method
cpg	385.92	J/mol×K	661.09	Joback Method
cpg	400.04	J/mol×K	699.89	Joback Method
cpg	413.48	J/mol×K	738.69	Joback Method
cpg	426.39	J/mol×K	777.48	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=R336499&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R336499&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>ripol:</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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