

# Ent- agathic acid methyl ester

<b>Inchi:</b>	InChI=1S/C21H32O4/c1-14(13-19(22)24-4)8-10-17-15(2)9-11-18-16(20(23)25-5)7-6-12-2
<b>InchiKey:</b>	MLSGWHAHBQGEBV-QAMHRUCZSA-N
<b>Formula:</b>	C21H32O4
<b>SMILES:</b>	<chem>C=C1CCC2C(C(=O)OC)CCCC2(C)C1CCC(C)=CC(=O)OC</chem>
<b>Mol. weight [g/mol]:</b>	348.48

## Physical Properties

Property code	Value	Unit	Source
gf	-164.96	kJ/mol	Joback Method
hf	-679.18	kJ/mol	Joback Method
hfus	37.17	kJ/mol	Joback Method
hvap	79.59	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.448		Crippen Method
mvol	291.310	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rmpol	2553.00		NIST Webbook
rmpol	2553.00		NIST Webbook
tb	857.12	K	Joback Method
tc	1074.29	K	Joback Method
tf	502.61	K	Joback Method
vc	1.103	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.46	J/molxK	857.12	Joback Method
cpg	984.53	J/molxK	893.32	Joback Method
cpg	1004.76	J/molxK	929.51	Joback Method
cpg	1024.29	J/molxK	965.71	Joback Method
cpg	1043.24	J/molxK	1001.90	Joback Method
cpg	1061.73	J/molxK	1038.10	Joback Method
cpg	1079.91	J/molxK	1074.29	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R519392&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R519392&amp;Units=SI</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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