

# 17«alpha»(H),21«beta»(H)-Bishomohopanoic acid methyl ester

<b>Inchi:</b>	InChI=1S/C33H56O2/c1-22(10-13-28(34)35-8)23-14-19-30(4)24(23)15-20-32(6)26(30)11
<b>InchiKey:</b>	ORWUNXLWVUEFW-VDXCZSIDSA-N
<b>Formula:</b>	C33H56O2
<b>SMILES:</b>	COC(=O)CCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
<b>Mol. weight [g/mol]:</b>	484.80

## Physical Properties

Property code	Value	Unit	Source
gf	155.77	kJ/mol	Joback Method
hf	-672.99	kJ/mol	Joback Method
hfus	32.43	kJ/mol	Joback Method
hvap	91.12	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	9.067		Crippen Method
mcvol	428.970	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
rinsol	3684.00		NIST Webbook
tb	1067.46	K	Joback Method
tc	1314.47	K	Joback Method
tf	685.71	K	Joback Method
vc	1.623	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1803.86	J/mol×K	1067.46	Joback Method
cpg	1868.10	J/mol×K	1108.63	Joback Method
cpg	1938.24	J/mol×K	1149.80	Joback Method
cpg	2015.12	J/mol×K	1190.96	Joback Method
cpg	2099.56	J/mol×K	1232.13	Joback Method
cpg	2192.41	J/mol×K	1273.30	Joback Method
cpg	2294.48	J/mol×K	1314.47	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=R418992&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R418992&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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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