

# allo-Cholanic (5«alpha») acid, methyl ester

<b>Inchi:</b>	InChI=1S/C25H42O5/c1-14(5-8-22(29)30-4)17-6-7-18-23-19(13-21(28)25(17,18)3)24(2)1
<b>InchiKey:</b>	DLYVTEULDNMQAR-BKTGEOEISA-N
<b>Formula:</b>	C25H42O5
<b>SMILES:</b>	COC(=O)CCC(C)C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CC(O)C12C
<b>Mol. weight [g/mol]:</b>	422.60

## Physical Properties

Property code	Value	Unit	Source
gf	-361.94	kJ/mol	Joback Method
hf	-1097.26	kJ/mol	Joback Method
hfus	47.90	kJ/mol	Joback Method
hvap	126.40	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.537		Crippen Method
mcvol	344.720	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	2941.00		NIST Webbook
rinpol	2941.00		NIST Webbook
rinpol	2941.00		NIST Webbook
ripol	3580.00		NIST Webbook
ripol	3580.00		NIST Webbook
tb	1144.56	K	Joback Method
tc	1412.67	K	Joback Method
tf	687.65	K	Joback Method
vc	1.288	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.41	J/molxK	1144.56	Joback Method
cpg	1514.54	J/molxK	1189.24	Joback Method
cpg	1557.15	J/molxK	1233.93	Joback Method
cpg	1602.74	J/molxK	1278.61	Joback Method
cpg	1651.80	J/molxK	1323.30	Joback Method

cpg	1704.82	J/mol×K	1367.98	Joback Method
cpg	1762.30	J/mol×K	1412.67	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=R533249&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R533249&amp;Units=SI</a>
<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.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>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>rinpol:</b>	Non-polar retention indices
<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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