

# 3«alpha»,6«beta»,7«beta»,12«alpha»-Tetrahydrox acid, acetate-methyl ester

InChI: InChI=1S/C33H50O10/c1-17/9-12-28(38)39-8)23-10-11-24-29-25(16-27(33(23,24)7)41-1  
InChIKey: NDZQWHMQQJJDYRD-QMMSOFMJSA-N

Formula: C33H50O10

SMILES: COC(=O)CCC(C)C1CCC2C3C(OC(C)=O)C(OC(C)=O)C4CC(OC(C)=O)CCC4(C)C3CC(

Mol. weight [g/mol]: 606.74

## Physical Properties

Property code	Value	Unit	Source
gf	-827.51	kJ/mol	Joback Method
hf	-1805.23	kJ/mol	Joback Method
hfus	68.58	kJ/mol	Joback Method
hvap	130.49	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	4.791		Crippen Method
mcvol	469.590	ml/mol	McGowan Method
pc	753.08	kPa	Joback Method
rinpol	3615.00		NIST Webbook
rinpol	3615.00		NIST Webbook
tb	1351.55	K	Joback Method
tc	1693.42	K	Joback Method
tf	879.75	K	Joback Method
vc	1.774	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2042.51	J/molxK	1351.55	Joback Method
cpg	2094.96	J/molxK	1408.53	Joback Method
cpg	2150.91	J/molxK	1465.51	Joback Method
cpg	2211.16	J/molxK	1522.48	Joback Method
cpg	2276.49	J/molxK	1579.46	Joback Method
cpg	2347.67	J/molxK	1636.44	Joback Method
cpg	2425.51	J/molxK	1693.42	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.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=R182351&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R182351&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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