

# 5«alpha»-Hydroxymarsupellyl acetate

**Inchi:** InChI=1S/C19H28O4/c1-10-13-14-15(19(13,6)9-7-8-18(14,4)5)17(23-12(3)21)16(10)22-1  
**InchiKey:** SYNMREOKVHJLFP-KZJPTANXSA-N  
**Formula:** C19H28O4  
**SMILES:** C=C1C(OC(C)=O)C(OC(C)=O)C2C3C1C2(C)CCCC3(C)C  
**Mol. weight [g/mol]:** 320.42

## Physical Properties

Property code	Value	Unit	Source
gf	-189.43	kJ/mol	Joback Method
hf	-685.65	kJ/mol	Joback Method
hfus	31.27	kJ/mol	Joback Method
hvap	72.90	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.498		Crippen Method
mcvol	256.570	ml/mol	McGowan Method
pc	1558.58	kPa	Joback Method
rinqol	1856.00		NIST Webbook
tb	796.42	K	Joback Method
tc	1014.11	K	Joback Method
tf	539.51	K	Joback Method
vc	0.979	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.15	J/molxK	796.42	Joback Method
cpg	866.94	J/molxK	832.70	Joback Method
cpg	888.41	J/molxK	868.98	Joback Method
cpg	909.79	J/molxK	905.27	Joback Method
cpg	931.29	J/molxK	941.55	Joback Method
cpg	953.13	J/molxK	977.83	Joback Method
cpg	975.55	J/molxK	1014.11	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=R561714&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R561714&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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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