

# 5-Androsten-17-one, 19-hydroxy-3b-methoxy-, methanesulfonate

Inchi:	InChI=1S/C21H32O5S/c1-20-10-9-18-16(17(20)6-7-19(20)22)5-4-14-12-15(25-2)8-11-21
InchiKey:	YECDAUWXRFWPSS-UHFFFAOYSA-N
Formula:	C21H32O5S
SMILES:	COC1CCC2(COS(C)(=O)=O)C(=CCC3C4CCC(=O)C4(C)CCC32)C1
Mol. weight [g/mol]:	396.54
CAS:	6494-00-4

## Physical Properties

Property code	Value	Unit	Source
gf	-498.76	kJ/mol	Joback Method
hf	-1035.75	kJ/mol	Joback Method
hfus	35.83	kJ/mol	Joback Method
hvap	88.59	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.490		Crippen Method
mcvol	300.410	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
tb	883.91	K	Joback Method
tc	1116.76	K	Joback Method
tf	584.43	K	Joback Method
vc	1.149	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1054.08	J/molxK	883.91	Joback Method
cpg	1079.59	J/molxK	922.72	Joback Method
cpg	1104.75	J/molxK	961.53	Joback Method
cpg	1129.80	J/molxK	1000.34	Joback Method
cpg	1155.00	J/molxK	1039.14	Joback Method
cpg	1180.59	J/molxK	1077.95	Joback Method
cpg	1206.84	J/molxK	1116.76	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6494004&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6494004&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

# 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>hvap:</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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