

# 5«beta»-Pregnan-3«alpha»,17«alpha»,20«beta»-tr

InChI: InChI=1S/C23H38O3/c1-14-23(26-21(2,3)25-14)12-10-20-19-7-5-15-13-16(24)6-8-17(15)  
17,20-acetonide  
InchiKey: AEYQWMMCYCJLEE-QUJHUTGTSA-N

Formula: C23H38O3

SMILES: CC1OC(C)(C)OC12CCC1C3CCC4CC(O)CCC4C3CCC12C

Mol. weight [g/mol]: 362.55

## Physical Properties

Property code	Value	Unit	Source
gf	9.85	kJ/mol	Joback Method
hf	-663.22	kJ/mol	Joback Method
hfus	39.91	kJ/mol	Joback Method
hvap	88.09	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	4.910		Crippen Method
mcvol	298.240	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	2665.00		NIST Webbook
rinpol	2665.00		NIST Webbook
tb	908.41	K	Joback Method
tc	1141.28	K	Joback Method
tf	582.01	K	Joback Method
vc	1.111	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1151.23	J/molxK	908.41	Joback Method
cpg	1183.04	J/molxK	947.22	Joback Method
cpg	1216.03	J/molxK	986.03	Joback Method
cpg	1250.67	J/molxK	1024.85	Joback Method
cpg	1287.41	J/molxK	1063.66	Joback Method
cpg	1326.73	J/molxK	1102.47	Joback Method
cpg	1369.09	J/molxK	1141.28	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R525154&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R525154&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>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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</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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