

# 21-Acetoxy-11beta,17alpha,20alpha-trihydroxypre

<b>Inchi:</b>	InChI=1S/C23H32O6/c1-13(24)29-12-19(27)23(28)9-7-17-16-5-4-14-10-15(25)6-8-21(14)
<b>InchiKey:</b>	TYKFSLOWQCQNQJ-MXUWMZRMSA-N
<b>Formula:</b>	C23H32O6
<b>SMILES:</b>	CC(=O)OCC(O)C1(O)CCC2C3CCC4=CC(=O)C=CC4(C)C3C(O)CC21C
<b>Mol. weight [g/mol]:</b>	404.50
<b>CAS:</b>	2871-71-8

## Physical Properties

Property code	Value	Unit	Source
gf	-433.44	kJ/mol	Joback Method
hf	-1013.33	kJ/mol	Joback Method
hfus	34.78	kJ/mol	Joback Method
hvap	127.22	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	1.920		Crippen Method
mcvol	309.510	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
tb	1184.17	K	Joback Method
tc	1454.37	K	Joback Method
tf	783.99	K	Joback Method
vc	1.157	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.83	J/molxK	1184.17	Joback Method
cpg	1400.90	J/molxK	1229.20	Joback Method
cpg	1459.34	J/molxK	1274.24	Joback Method
cpg	1523.78	J/molxK	1319.27	Joback Method
cpg	1594.86	J/molxK	1364.30	Joback Method
cpg	1673.21	J/molxK	1409.34	Joback Method
cpg	1759.45	J/molxK	1454.37	Joback Method

# Sources

<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=C2871718&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2871718&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>

# 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>mcvol:</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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