

# 3,17-Dimethoxypregna-2,4-dien-20-one

<b>Inchi:</b>	InChI=1S/C23H34O3/c1-15(24)23(26-5)13-10-20-18-7-6-16-14-17(25-4)8-11-21(16,2)19
<b>InchiKey:</b>	WGMORNSWMKZSGW-UHFFFAOYSA-N
<b>Formula:</b>	C23H34O3
<b>SMILES:</b>	<chem>COC1=CCC2(C)C(=C1)CCC1C2CCC2(C)C1CCC2(OC)C(C)=O</chem>
<b>Mol. weight [g/mol]:</b>	358.51

## Physical Properties

Property code	Value	Unit	Source
gf	-4.87	kJ/mol	Joback Method
hf	-537.01	kJ/mol	Joback Method
hfus	26.26	kJ/mol	Joback Method
hvap	76.71	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.064		Crippen Method
mvol	296.200	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinpol	2959.60		NIST Webbook
rinpol	2959.60		NIST Webbook
tb	872.32	K	Joback Method
tc	1110.16	K	Joback Method
tf	587.30	K	Joback Method
vc	1.117	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.14	J/mol×K	872.32	Joback Method
cpg	1058.14	J/mol×K	911.96	Joback Method
cpg	1088.04	J/mol×K	951.60	Joback Method
cpg	1119.28	J/mol×K	991.24	Joback Method
cpg	1152.31	J/mol×K	1030.88	Joback Method
cpg	1187.58	J/mol×K	1070.52	Joback Method
cpg	1225.52	J/mol×K	1110.16	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U333779&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333779&amp;Units=SI</a>
<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>

# 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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