

# .beta.-Estradiol, dimethyl ether

<b>Other names:</b>	Estra-1,3,5(10)-triene, 3,17-dimethoxy-, (17«beta»)-
<b>Inchi:</b>	InChI=1S/C20H28O2/c1-20-11-10-16-15-7-5-14(21-2)12-13(15)4-6-17(16)18(20)8-9-19(2)
<b>InchiKey:</b>	UJVDXOJUUSHVJY-UHFFFAOYSA-N
<b>Formula:</b>	C20H28O2
<b>SMILES:</b>	COc1ccc2c(c1)CCC1C2CCC2(C)C(OC)CCC12
<b>Mol. weight [g/mol]:</b>	300.44
<b>CAS:</b>	4954-14-7

## Physical Properties

Property code	Value	Unit	Source
gf	137.81	kJ/mol	Joback Method
hf	-326.34	kJ/mol	Joback Method
hfus	29.24	kJ/mol	Joback Method
hvap	66.85	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.566		Crippen Method
mcvol	248.060	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	2580.40		NIST Webbook
tb	758.14	K	Joback Method
tc	990.15	K	Joback Method
tf	473.28	K	Joback Method
vc	0.934	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.40	J/molxK	758.14	Joback Method
cpg	817.68	J/molxK	796.81	Joback Method
cpg	839.89	J/molxK	835.48	Joback Method
cpg	861.21	J/molxK	874.14	Joback Method
cpg	881.86	J/molxK	912.81	Joback Method
cpg	902.03	J/molxK	951.48	Joback Method
cpg	921.91	J/molxK	990.15	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4954147&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4954147&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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