

# 17«beta»-Oestradiol, 3-methoxy, TFA

<b>Inchi:</b>	InChI=1S/C21H25F3O3/c1-20-10-9-15-14-6-4-13(26-2)11-12(14)3-5-16(15)17(20)7-8-18
<b>InchiKey:</b>	RBZLYLXZTKIMFG-AUFNPSFISA-N
<b>Formula:</b>	C21H25F3O3
<b>SMILES:</b>	COc1ccc2c(c1)CCC1C2CCC2(C)C(OC(=O)C(F)(F)F)CCC12
<b>Mol. weight [g/mol]:</b>	382.42

## Physical Properties

Property code	Value	Unit	Source
gf	-564.28	kJ/mol	Joback Method
hf	-1056.64	kJ/mol	Joback Method
hfus	35.26	kJ/mol	Joback Method
hvap	72.07	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.025		Crippen Method
mvol	269.030	ml/mol	McGowan Method
pc	1478.15	kPa	Joback Method
rinpol	2390.00		NIST Webbook
rinpol	2422.00		NIST Webbook
tb	829.47	K	Joback Method
tc	1049.30	K	Joback Method
tf	538.67	K	Joback Method
vc	1.040	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.66	J/molxK	829.47	Joback Method
cpg	921.65	J/molxK	866.11	Joback Method
cpg	940.94	J/molxK	902.75	Joback Method
cpg	959.74	J/molxK	939.39	Joback Method
cpg	978.22	J/molxK	976.02	Joback Method
cpg	996.60	J/molxK	1012.66	Joback Method
cpg	1015.06	J/molxK	1049.30	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=R523905&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R523905&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>rinpola:</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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