

# 17«beta»-Oestradiol, 2-methoxy, TFA

<b>Inchi:</b>	InChI=1S/C23H24F6O5/c1-21-8-7-12-13(15(21)5-6-18(21)34-20(31)23(27,28)29)4-3-11-
<b>InchiKey:</b>	VEIPLNGOHCVRDA-BYSRFSNKSA-N
<b>Formula:</b>	C23H24F6O5
<b>SMILES:</b>	COc1cc2c(cc1OC(=O)C(F)(F)F)CCC1C2CCC2(C)C(OC(=O)C(F)(F)F)CCC12
<b>Mol. weight [g/mol]:</b>	494.42

## Physical Properties

Property code	Value	Unit	Source
gf	-1372.58	kJ/mol	Joback Method
hf	-1951.27	kJ/mol	Joback Method
hfus	44.66	kJ/mol	Joback Method
hvap	82.60	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.493		Crippen Method
mcvol	309.960	ml/mol	McGowan Method
pc	1207.31	kPa	Joback Method
rinpol	2505.00		NIST Webbook
rinpol	2474.00		NIST Webbook
rinpol	2474.00		NIST Webbook
tb	951.08	K	Joback Method
tc	1169.77	K	Joback Method
tf	650.08	K	Joback Method
vc	1.218	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1095.57	J/molxK	951.08	Joback Method
cpg	1114.26	J/molxK	987.53	Joback Method
cpg	1132.73	J/molxK	1023.98	Joback Method
cpg	1151.18	J/molxK	1060.43	Joback Method
cpg	1169.82	J/molxK	1096.87	Joback Method
cpg	1188.84	J/molxK	1133.32	Joback Method
cpg	1208.45	J/molxK	1169.77	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R523881&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R523881&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>hvpap:</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>rinppl:</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

Latest version available from:

<https://www.chemeo.com/cid/33-112-0/17-beta-Oestradiol-2-methoxy-TFA.pdf>

Generated by Cheméo on 2024-04-25 16:17:16.544016033 +0000 UTC m=+16351085.464593348.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.