

# 16-epi-Oestriol, TFA

<b>Inchi:</b>	InChI=1S/C24H21F9O6/c1-21-7-6-13-12-5-3-11(37-18(34)22(25,26)27)8-10(12)2-4-14(1
<b>InchiKey:</b>	WWJXNFAAIBBBGC-BZEWANASA-N
<b>Formula:</b>	C24H21F9O6
<b>SMILES:</b>	CC12CCC3c4ccc(OC(=O)C(F)(F)F)cc4CCC3C1CC(OC(=O)C(F)(F)F)C2OC(=O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	576.41

## Physical Properties

Property code	Value	Unit	Source
gf	-2072.75	kJ/mol	Joback Method
hf	-2690.44	kJ/mol	Joback Method
hfus	52.14	kJ/mol	Joback Method
hvap	86.85	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	5.568		Crippen Method
mcvol	330.930	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
rinpol	2459.00		NIST Webbook
rinpol	2459.00		NIST Webbook
rinpol	2500.00		NIST Webbook
tb	1012.76	K	Joback Method
tc	1239.90	K	Joback Method
tf	698.71	K	Joback Method
vc	1.323	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1199.91	J/molxK	1012.76	Joback Method
cpg	1218.65	J/molxK	1050.62	Joback Method
cpg	1237.57	J/molxK	1088.47	Joback Method
cpg	1256.91	J/molxK	1126.33	Joback Method
cpg	1276.93	J/molxK	1164.19	Joback Method
cpg	1297.87	J/molxK	1202.05	Joback Method
cpg	1320.00	J/molxK	1239.90	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R523836&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R523836&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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