

# 3«beta»-Hydroxy-5«alpha»-estran-16-one, TFA

<b>Inchi:</b>	InChI=1S/C20H27F3O3/c1-19-7-6-15-14-5-3-13(26-18(25)20(21,22)23)8-11(14)2-4-16(1
<b>InchiKey:</b>	GNIHRIPHOVZFN-LCGHUAIBSA-N
<b>Formula:</b>	C20H27F3O3
<b>SMILES:</b>	CC12CCC3C4CCC(OC(=O)C(F)(F)F)CC4CCC3C1CC(=O)C2
<b>Mol. weight [g/mol]:</b>	372.42

## Physical Properties

Property code	Value	Unit	Source
gf	-666.70	kJ/mol	Joback Method
hf	-1221.09	kJ/mol	Joback Method
hfus	30.63	kJ/mol	Joback Method
hvap	68.20	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.682		Crippen Method
mvol	263.540	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	2303.00		NIST Webbook
rinpol	2369.00		NIST Webbook
tb	830.23	K	Joback Method
tc	1057.36	K	Joback Method
tf	525.07	K	Joback Method
vc	1.012	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.84	J/mol×K	830.23	Joback Method
cpg	963.52	J/mol×K	868.08	Joback Method
cpg	985.15	J/mol×K	905.94	Joback Method
cpg	1005.93	J/mol×K	943.79	Joback Method
cpg	1026.05	J/mol×K	981.65	Joback Method
cpg	1045.72	J/mol×K	1019.50	Joback Method
cpg	1065.12	J/mol×K	1057.36	Joback Method

# Sources

<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=R523950&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R523950&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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