

# Estrone, TFA

<b>Inchi:</b>	InChI=1S/C20H21F3O3/c1-19-9-8-14-13-5-3-12(26-18(25)20(21,22)23)10-11(13)2-4-15(
<b>InchiKey:</b>	UAPVNSRFPMGHBC-ZEPBGEJQSA-N
<b>Formula:</b>	C20H21F3O3
<b>SMILES:</b>	CC12CCC3c4ccc(OC(=O)C(F)(F)F)cc4CCC3C1CCC2=O
<b>Mol. weight [g/mol]:</b>	366.37

## Physical Properties

Property code	Value	Unit	Source
gf	-582.58	kJ/mol	Joback Method
hf	-1021.14	kJ/mol	Joback Method
hfus	29.92	kJ/mol	Joback Method
hvap	71.99	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.579		Crippen Method
mcvol	250.640	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinqol	2392.00		NIST Webbook
tb	856.66	K	Joback Method
tc	1090.57	K	Joback Method
tf	577.63	K	Joback Method
vc	0.974	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.26	J/molxK	856.66	Joback Method
cpg	863.43	J/molxK	895.65	Joback Method
cpg	882.05	J/molxK	934.63	Joback Method
cpg	900.33	J/molxK	973.62	Joback Method
cpg	918.51	J/molxK	1012.60	Joback Method
cpg	936.79	J/molxK	1051.59	Joback Method
cpg	955.41	J/molxK	1090.57	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=R293877&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R293877&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>
<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>

# 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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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