

# 5-Pregnen-3-«beta»,20-«beta»-diol, TFA

<b>Inchi:</b>	InChI=1S/C25H32F6O4/c1-13(34-20(32)24(26,27)28)17-6-7-18-16-5-4-14-12-15(35-21(3
<b>InchiKey:</b>	CEUTXEHQJLYLFE-JHLVREFVSA-N
<b>Formula:</b>	C25H32F6O4
<b>SMILES:</b>	CC(OC(=O)C(F)(F)F)C1CCC2C3CC=C4CC(OC(=O)C(F)(F)F)CCC4(C)C3CCC12C
<b>Mol. weight [g/mol]:</b>	510.51

## Physical Properties

Property code	Value	Unit	Source
gf	-1305.12	kJ/mol	Joback Method
hf	-1972.20	kJ/mol	Joback Method
hfus	39.70	kJ/mol	Joback Method
hvap	79.91	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	6.534		Crippen Method
mcvol	340.870	ml/mol	McGowan Method
pc	1045.30	kPa	Joback Method
rinpola	2489.00		NIST Webbook
rinpola	2507.00		NIST Webbook
tb	951.62	K	Joback Method
tc	1170.61	K	Joback Method
tf	611.73	K	Joback Method
vc	1.331	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1264.21	J/molxK	951.62	Joback Method
cpg	1289.77	J/molxK	988.12	Joback Method
cpg	1315.84	J/molxK	1024.62	Joback Method
cpg	1342.73	J/molxK	1061.12	Joback Method
cpg	1370.78	J/molxK	1097.61	Joback Method
cpg	1400.27	J/molxK	1134.11	Joback Method
cpg	1431.54	J/molxK	1170.61	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=R385347&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R385347&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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