

# 5-«alpha»-Pregnan-3-«beta»,20-«beta»-diol, TFA

Inchi:	InChI=1S/C25H34F6O4/c1-13(34-20(32)24(26,27)28)17-6-7-18-16-5-4-14-12-15(35-21(3
InchiKey:	ZYWWYWQPOLCWDY-ZMNIESCDSA-N
Formula:	C25H34F6O4
SMILES:	CC(OC(=O)C(F)(F)F)C1CCC2C3CCC4CC(OC(=O)C(F)(F)F)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	512.53

## Physical Properties

Property code	Value	Unit	Source
gf	-1333.16	kJ/mol	Joback Method
hf	-2038.85	kJ/mol	Joback Method
hfus	39.94	kJ/mol	Joback Method
hvap	78.65	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.613		Crippen Method
mvol	345.170	ml/mol	McGowan Method
pc	1009.73	kPa	Joback Method
rinpol	2523.00		NIST Webbook
rinpol	2504.00		NIST Webbook
tb	942.81	K	Joback Method
tc	1159.83	K	Joback Method
tf	594.21	K	Joback Method
vc	1.343	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1297.92	J/molxK	942.81	Joback Method
cpg	1323.94	J/molxK	978.98	Joback Method
cpg	1350.26	J/molxK	1015.15	Joback Method
cpg	1377.20	J/molxK	1051.32	Joback Method
cpg	1405.06	J/molxK	1087.49	Joback Method
cpg	1434.12	J/molxK	1123.66	Joback Method
cpg	1464.71	J/molxK	1159.83	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=R385025&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R385025&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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