

# 1,3,5(10)-Oestratriene-2-methoxy-3,16«alpha»,17«beta»-trifluoromethyl-16,17-PFP

InChI: InChI=1S/C25H24F10O6/c1-21-6-5-11-12(4-3-10-7-15(36)16(39-2)8-13(10)11)14(21)9-10  
InChIKey: XKCPQLZEMXYPPS-CBPXGTFBSA-N

Formula: C25H24F10O6

SMILES: COc1cc2c(cc1O)CCC1C2CCC2(C)C1CC(OC(=O)C(F)(F)C(F)(F)F)C2OC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 610.44

## Physical Properties

Property code	Value	Unit	Source
gf	-2282.00	kJ/mol	Joback Method
hf	-2980.67	kJ/mol	Joback Method
hfus	54.58	kJ/mol	Joback Method
hvap	93.23	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.086		Crippen Method
mcvol	351.090	ml/mol	McGowan Method
pc	1053.46	kPa	Joback Method
rinpol	2544.00		NIST Webbook
tb	1058.43	K	Joback Method
tc	1296.63	K	Joback Method
tf	774.78	K	Joback Method
vc	1.345	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1321.07	J/molxK	1058.43	Joback Method
cpg	1345.22	J/molxK	1098.13	Joback Method
cpg	1370.68	J/molxK	1137.83	Joback Method
cpg	1397.82	J/molxK	1177.53	Joback Method
cpg	1427.04	J/molxK	1217.23	Joback Method
cpg	1458.69	J/molxK	1256.93	Joback Method
cpg	1493.17	J/molxK	1296.63	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=R537132&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R537132&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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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