

# Estrone, pentafluoropropionate

<b>Inchi:</b>	InChI=1S/C21H21F5O3/c1-19-9-8-14-13-5-3-12(29-18(28)20(22,23)21(24,25)26)10-11(1
<b>InchiKey:</b>	VUGNDDMASKYDDH-UHFFFAOYSA-N
<b>Formula:</b>	C21H21F5O3
<b>SMILES:</b>	CC12CCC3c4ccc(OC(=O)C(F)(F)C(F)(F)F)cc4CCC3C1CCC2=O
<b>Mol. weight [g/mol]:</b>	416.38

## Physical Properties

Property code	Value	Unit	Source
gf	-960.94	kJ/mol	Joback Method
hf	-1442.75	kJ/mol	Joback Method
hfus	31.26	kJ/mol	Joback Method
hvap	71.29	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.215		Crippen Method
mcvol	268.270	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	2458.50		NIST Webbook
tb	874.85	K	Joback Method
tc	1100.58	K	Joback Method
tf	592.50	K	Joback Method
vc	1.054	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.28	J/molxK	874.85	Joback Method
cpg	937.86	J/molxK	912.47	Joback Method
cpg	956.01	J/molxK	950.09	Joback Method
cpg	973.97	J/molxK	987.71	Joback Method
cpg	991.96	J/molxK	1025.33	Joback Method
cpg	1010.22	J/molxK	1062.95	Joback Method
cpg	1028.98	J/molxK	1100.58	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U352217&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352217&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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