

# Fluoromethalone

<b>Other names:</b>	17-acetyl-9-fluoro-11,17-dihydroxy-6,10,13-trimethyl-6,7,8,11,12,14,15,16-octahydrocyclo
<b>Inchi:</b>	InChI=1S/C22H29FO4/c1-12-9-17-15-6-8-21(27,13(2)24)20(15,4)11-18(26)22(17,23)19(3
<b>InchiKey:</b>	FAOZLTXFLGPHNG-UHFFFAOYSA-N
<b>Formula:</b>	C22H29FO4
<b>SMILES:</b>	CC(=O)C1(O)CCC2C3CC(C)C4=CC(=O)C=CC4(C)C3(F)C(O)CC21C
<b>Mol. weight [g/mol]:</b>	376.47

## Physical Properties

Property code	Value	Unit	Source
gf	-405.61	kJ/mol	Joback Method
hf	-904.17	kJ/mol	Joback Method
hfus	28.29	kJ/mol	Joback Method
hvap	104.02	kJ/mol	Joback Method
log10ws	-4.10		Aqueous Solubility Prediction Method
log10ws	-4.10		Estimated Solubility Method
logp	2.923		Crippen Method
mcvol	285.450	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
tb	1041.97	K	Joback Method
tc	1280.56	K	Joback Method
tf	724.92	K	Joback Method
vc	1.085	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1145.02	J/molxK	1041.97	Joback Method
cpg	1186.53	J/molxK	1081.74	Joback Method
cpg	1232.16	J/molxK	1121.50	Joback Method
cpg	1282.44	J/molxK	1161.27	Joback Method
cpg	1337.93	J/molxK	1201.03	Joback Method
cpg	1399.19	J/molxK	1240.80	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>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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