

# Flufenamic acid, methyl ester

<b>Other names:</b>	Methyl 2-pyrrol[3-(trifluoromethyl)phenyl]aminomorphobenzoate Flufenamic acid, methyl deriv.
<b>Inchi:</b>	InChI=1S/C15H12F3NO2/c1-21-14(20)12-7-2-3-8-13(12)19-11-6-4-5-10(9-11)15(16,17)1
<b>InchiKey:</b>	CACWGXKXXWFHZRW-UHFFFAOYSA-N
<b>Formula:</b>	C15H12F3NO2
<b>SMILES:</b>	<chem>COC(=O)c1ccccc1Nc1cccc(C(F)(F)F)c1</chem>
<b>Mol. weight [g/mol]:</b>	295.26

## Physical Properties

Property code	Value	Unit	Source
gf	-445.14	kJ/mol	Joback Method
hf	-691.22	kJ/mol	Joback Method
hfus	31.62	kJ/mol	Joback Method
hvap	66.70	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.236		Crippen Method
mcvol	197.420	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1875.00		NIST Webbook
rinpol	1915.40		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1915.40		NIST Webbook
tb	726.96	K	Joback Method
tc	946.77	K	Joback Method
tf	465.70	K	Joback Method
vc	0.761	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.86	J/molxK	726.96	Joback Method
cpg	555.88	J/molxK	763.59	Joback Method
cpg	567.85	J/molxK	800.23	Joback Method
cpg	578.82	J/molxK	836.86	Joback Method

cpg	588.85	J/mol×K	873.50	Joback Method
cpg	598.01	J/mol×K	910.13	Joback Method
cpg	606.36	J/mol×K	946.77	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=U333177&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333177&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>

## 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>mvol:</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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