

# Flurazepam M (hydroxyethyl-), hydrolysis, acetylated

Inchi:	InChI=1S/C19H17ClFNO4/c1-12(23)22(9-10-26-13(2)24)18-8-7-14(20)11-16(18)19(25)1
InchiKey:	MBVCFUQVKXBRED-UHFFFAOYSA-N
Formula:	C19H17ClFNO4
SMILES:	CC(=O)OCCN(C(C)=O)c1ccc(Cl)cc1C(=O)c1ccccc1F
Mol. weight [g/mol]:	377.79

## Physical Properties

Property code	Value	Unit	Source
gf	-282.69	kJ/mol	Joback Method
hf	-611.12	kJ/mol	Joback Method
hfus	48.16	kJ/mol	Joback Method
hvap	92.68	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.626		Crippen Method
mcvol	265.620	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
tb	935.59	K	Joback Method
tc	1165.39	K	Joback Method
tf	629.29	K	Joback Method
vc	1.004	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.96	J/molxK	935.59	Joback Method
cpg	785.66	J/molxK	973.89	Joback Method
cpg	795.24	J/molxK	1012.19	Joback Method
cpg	803.76	J/molxK	1050.49	Joback Method
cpg	811.26	J/molxK	1088.79	Joback Method
cpg	817.80	J/molxK	1127.09	Joback Method
cpg	823.44	J/molxK	1165.39	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R313070&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R313070&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>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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