Flunitrazepam M (noramino-), hydrolysis, acetylated

Inchi: InChI=1S/C17H15FN2O3/c1-10(21)19-12-7-8-16(20-11(2)22)14(9-12)17(23)13-5-3-4-6-1

InchiKey: BBAPQKFIQPMGGA-UHFFFAOYSA-N

Formula: C17H15FN2O3

SMILES: CC(O)=Nc1ccc(N=C(C)O)c(C(=O)c2ccccc2F)c1

Mol. weight [g/mol]: 314.31

Physical Properties

Property code	Value	Unit	Source
hf	-423.85	kJ/mol	Joback Method
hvap	106.05	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.272		Crippen Method
mcvol	229.310	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	2715.00		NIST Webbook
tb	1047.28	K	Joback Method
tc	1286.71	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R313030&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature