Flunitrazepam M (amino-), hydrolysis, acetylated

Inchi: InChI=1S/C18H17FN2O3/c1-11(22)20-13-8-9-17(21(3)12(2)23)15(10-13)18(24)14-6-4-5-

InchiKey: SUUGLAZBOARLSU-UHFFFAOYSA-N

Formula: C18H17FN2O3

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

Mol. weight [g/mol]: 328.34

Physical Properties

Property code	Value	Unit	Source
gf	-84.79	kJ/mol	Joback Method
hf	-389.05	kJ/mol	Joback Method
hfus	45.29	kJ/mol	Joback Method
hvap	90.10	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.998		Crippen Method
mcvol	243.400	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	2870.00		NIST Webbook
rinpol	2870.00		NIST Webbook
tb	903.03	K	Joback Method
tc	1132.66	K	Joback Method
tf	618.53	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.76	J/mol×K	903.03	Joback Method
cpg	735.24	J/mol×K	941.30	Joback Method
cpg	745.68	J/mol×K	979.57	Joback Method
cpg	755.13	J/mol×K	1017.85	Joback Method
cpg	763.68	J/mol×K	1056.12	Joback Method
cpg	771.39	J/mol×K	1094.39	Joback Method
cpg	778.32	J/mol×K	1132.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313025&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume