

Flurazepam M (bisdeseethyl-)-H2O, hydrolysis, acetylated

Inchi:	InChI=1S/C19H18ClFN2O3/c1-12(24)22-9-10-23(13(2)25)18-8-7-14(20)11-16(18)19(26)
InchiKey:	DWCBOQDXAIRNCQ-UHFFFAOYSA-N
Formula:	C19H18ClFN2O3
SMILES:	CC(=O)N(CCN=C(C)O)c1ccc(Cl)cc1C(=O)c1ccccc1F
Mol. weight [g/mol]:	376.81

Physical Properties

Property code	Value	Unit	Source
hf	-446.12	kJ/mol	Joback Method
hvap	103.60	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.039		Crippen Method
mcpvol	269.730	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tb	1028.04	K	Joback Method
tc	1264.52	K	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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