Midazolam M (hydroxy-), acetylated

Inchi: InChI=1S/C19H14ClFN4O2/c1-10-23-24-18-19(27-11(2)26)22-17(13-5-3-4-6-15(13)21)14
InchiKey: DDIJYCPUZHDGPP-UHFFFAOYSA-N
Formula: C19H14ClFN4O2
SMILES: CC(=O)OC1N=C(c2ccccc2F)c2cc(Cl)ccc2-n2c(C)nnc21
Mol. weight [g/mol]: 384.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.45		Crippen Method
logp	3.781		Crippen Method
mcvol	257.800	ml/mol	McGowan Method
rinpol	2820.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R313307&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices