N-Desmethylflunitrazepam, trimethylsilyl derivative

Inchi: InChI=1S/C18H18FN3O3Si/c1-26(2,3)25-17-11-20-18(13-6-4-5-7-15(13)19)14-10-12(22(

InchiKey: WJKWHPXTZPEKFR-UHFFFAOYSA-N

Formula: C18H18FN3O3Si

SMILES: C[Si](C)(C)OC1=Nc2ccc([N+](=O)[O-])cc2C(c2ccccc2F)=NC1

Mol. weight [g/mol]: 371.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	4.466		Crippen Method
rinpol	2538.60		NIST Webbook
rinpol	2538.60		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U417192&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices