Ftorafur, TMS

Inchi: InChI=1S/C11H17FN2O3Si/c1-18(2,3)17-10-8(12)7-14(11(15)13-10)9-5-4-6-16-9/h7,9H,
InchiKey: STWOABMRTGNUOL-UHFFFAOYSA-N
Formula: C11H17FN2O3Si
SMILES: C[Si](C)(C)Oc1nc(=O)n(C2CCCO2)cc1F
Mol. weight [g/mol]: 272.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.54		Crippen Method
logp	1.905		Crippen Method
rinpol	1318.70		NIST Webbook
rinpol	1318.70		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R245279&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices