2(3H)-Furanone, TMS (possibly, MSTFA-adduct)

Inchi: InChI=1S/C10H18F3NO3Si/c1-14(8(15)10(11,12)13)9(6-5-7-16-9)17-18(2,3)4/h5-7H2,1-

InchiKey: WJAADKYCKYZLPI-UHFFFAOYSA-N

Formula: C10H18F3NO3Si

SMILES: CN(C(=O)C(F)(F)F)C1(O[Si](C)(C)C)CCCO1

Mol. weight [g/mol]: 285.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.24		Crippen Method
logp	2.323		Crippen Method
rinpol	1778.00		NIST Webbook
rinpol	1778.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R631219&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

rinpol: Non-polar retention indices