1-Butanamine DMPFPS

Inchi: InChI=1S/C12H16F5NSi/c1-4-5-6-18-19(2,3)12-10(16)8(14)7(13)9(15)11(12)17/h18H,4-6
InchiKey: WSIXUEGTAWXHHQ-UHFFFAOYSA-N
Formula: C12H16F5NSi
SMILES: CCCCN[Si](C)(C)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 297.34
CAS: 71338-93-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.83		Crippen Method
logp	3.184		Crippen Method
rinpol	1280.00		NIST Webbook
rinpol	1280.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71338937&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