Niflumic acid tbdms

Other names: Niflumic acid, tbdms derivative
Inchi: InChI=1S/C19H23F3N2O2Si/c1-18(2,3)27(4,5)26-17(25)15-10-7-11-23-16(15)24-14-9-6-
InchiKey: ABVMYTKMQZELRT-UHFFFAOYSA-N
Formula: C19H23F3N2O2Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cccnc1Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 396.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	6.006		Crippen Method
rinpol	2335.60		NIST Webbook
rinpol	2335.60		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U331798&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