Trimethylsilyl 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitro-be

Inchi: InChI=1S/C17H15ClF3NO5Si/c1-28(2,3)27-16(23)12-9-11(5-6-14(12)22(24)25)26-15-7-4

InchiKey: LYBBQUWIIRSFIA-UHFFFAOYSA-N

Formula: C17H15ClF3NO5Si

SMILES: C[Si](C)(C)OC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]

Mol. weight [g/mol]: 433.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.68		Crippen Method
logp	6.051		Crippen Method
rinpol	2320.00		NIST Webbook
rinpol	2320.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U372988&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