

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/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/18-577-2/Trimethylsilyl-5-2-chloro-4-trifluoromethyl-phenoxy-2-nitro-benzoate.pdf>

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