8-Chlorooctyl trimethylsilyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, 8-chlorooctyl trimethylsilyl ester
Inchi: InChI=1S/C19H29ClO4Si/c1-25(2,3)24-19(22)17-13-9-8-12-16(17)18(21)23-15-11-7-5-4-
InchiKey: BRVPUSOIOFPHCP-UHFFFAOYSA-N
Formula: C19H29ClO4Si
SMILES: C[Si](C)(C)OC(=O)c1ccccc1C(=O)OCCCCCCCCCCl
Mol. weight [g/mol]: 384.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	5.414		Crippen Method
rinpol	2521.00		NIST Webbook
rinpol	2521.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373668&Units=SI

Legend

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