tert-Butyldimethylsilyl (Z)-non-3-enyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, (Z)-non-3-enyl tert-butyldimethylsilyl ester
Inchi: InChI=1S/C23H36O4Si/c1-7-8-9-10-11-12-15-18-26-21(24)19-16-13-14-17-20(19)22(25)
InchiKey: KZEGMMGPPBSCLD-QXMHVHEDSA-N
Formula: C23H36O4Si
SMILES: CCCCCC=CCCOC(=O)c1ccccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 404.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	6.532		Crippen Method
rinpol	2530.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373673&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