tert-Butyldimethylsilyl prop-2-ynyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, prop-2-ynyl tert-butyldimethylsilyl ester
Inchi: InChI=1S/C17H22O4Si/c1-7-12-20-15(18)13-10-8-9-11-14(13)16(19)21-22(5,6)17(2,3)4/h
InchiKey: QNVBAIAHWLUCDM-UHFFFAOYSA-N
Formula: C17H22O4Si
SMILES: C#CCOC(=O)c1ccccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 318.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	3.639		Crippen Method
rinpol	1974.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373519&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