tert-Butyldimethylsilyl heptyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, heptyl tert-butyldimethylsilyl ester
Inchi: InChI=1S/C21H34O4Si/c1-7-8-9-10-13-16-24-19(22)17-14-11-12-15-18(17)20(23)25-26(
InchiKey: MQIOYOONYWNPHH-UHFFFAOYSA-N
Formula: C21H34O4Si
SMILES: CCCCCCCOC(=O)c1ccccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 378.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	5.976		Crippen Method
rinpol	2348.00		NIST Webbook
rinpol	2348.00		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=U373647&Units=SI

Legend

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