(E)-3,7-Dimethylocta-2,6-dienyl trimethylsilyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, (E)-3,7-dimethylocta-2,6-dienyl trimethylsilyl ester
Inchi: InChI=1S/C21H30O4Si/c1-16(2)10-9-11-17(3)14-15-24-20(22)18-12-7-8-13-19(18)21(23
InchiKey: LQGCNXWJYMTBDN-SAPNQHFASA-N
Formula: C21H30O4Si
SMILES: CC(C)=CCCC(C)=CCOC(=O)c1ccccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 374.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.32		Crippen Method
logp	5.528		Crippen Method
rinpol	2404.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373511&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