

tert-Butyldimethylsilyl 3,7-dimethyloct-6-enyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 3,7-dimethyloct-6-enyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C24H38O4Si/c1-18(2)12-11-13-19(3)16-17-27-22(25)20-14-9-10-15-21(20)23(
InchiKey:	CQOWNGUPNVMRRS-UHFFFAOYSA-N
Formula:	C24H38O4Si
SMILES:	CC(C)=CCCC(C)CCOC(=O)c1cccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	418.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.48		Crippen Method
logp	6.778		Crippen Method
rinpol	2576.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373649&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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