

tert-Butyldimethylsilyl 3,5,5-trimethylhexyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 3,5,5-trimethylhexyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C23H38O4Si/c1-17(16-22(2,3)4)14-15-26-20(24)18-12-10-11-13-19(18)21(25)
InchiKey:	URVFLTXJZBJUAO-UHFFFAOYSA-N
Formula:	C23H38O4Si
SMILES:	CC(CCOC(=O)c1cccc1C(=O)O[Si](C)(C)C(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]:	406.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.97		Crippen Method
logp	6.468		Crippen Method
rinpol	2418.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373819&Units=SI

Legend

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

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