

tert-Butyldimethylsilyl 3-methylbutan-2-yl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 3-methylbutan-2-yl -tert-butyldimethylsilylsilyl ester
Inchi:	InChI=1S/C19H30O4Si/c1-13(2)14(3)22-17(20)15-11-9-10-12-16(15)18(21)23-24(7,8)19
InchiKey:	MHBVEYCQLDGQKB-UHFFFAOYSA-N
Formula:	C19H30O4Si
SMILES:	CC(C)C(C)OC(=O)c1ccccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	350.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.64		Crippen Method
logp	5.050		Crippen Method
rinpol	2065.00		NIST Webbook
rinpol	2065.00		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=U373640&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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