

tert-Butyldimethylsilyl neopentyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, neopentyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C19H30O4Si/c1-18(2,3)13-22-16(20)14-11-9-10-12-15(14)17(21)23-24(7,8)19
InchiKey:	LMTYOIQHBNNIPD-UHFFFAOYSA-N
Formula:	C19H30O4Si
SMILES:	CC(C)(C)COC(=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	-3.53		Crippen Method
logp	5.051		Crippen Method
rinpol	2038.00		NIST Webbook
rinpol	2038.00		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=U373502&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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<https://www.chemeo.com/cid/22-363-4/tert-Butyldimethylsilyl-neopentyl-phthalate.pdf>

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