

tert-Butyldimethylsilyl pentyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, pentyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C19H30O4Si/c1-7-8-11-14-22-17(20)15-12-9-10-13-16(15)18(21)23-24(5,6)19
InchiKey:	MQUBFYXVDVAYJY-UHFFFAOYSA-N
Formula:	C19H30O4Si
SMILES:	CCCCCOC(=O)c1cccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	350.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	5.196		Crippen Method
rinpol	2154.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373662&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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