

tert-Butyldimethylsilyl phenyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, phenyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C20H24O4Si/c1-20(2,3)25(4,5)24-19(22)17-14-10-9-13-16(17)18(21)23-15-11
InchiKey:	KHJPXYKYBZHYGD-UHFFFAOYSA-N
Formula:	C20H24O4Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)c1ccccc1C(=O)Oc1ccccc1
Mol. weight [g/mol]:	356.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.94		Crippen Method
logp	5.068		Crippen Method
rinpol	2365.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373818&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/40-144-7/tert-Butyldimethylsilyl-phenyl-phthalate.pdf>

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