

tert-Butyldimethylsilyl cyclohexyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, cyclohexyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C20H30O4Si/c1-20(2,3)25(4,5)24-19(22)17-14-10-9-13-16(17)18(21)23-15-11
InchiKey:	ALPPAKZSBMNTSE-UHFFFAOYSA-N
Formula:	C20H30O4Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)c1cccc1C(=O)OC1CCCCC1
Mol. weight [g/mol]:	362.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	5.338		Crippen Method
rinpol	2348.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373885&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/40-175-3/tert-Butyldimethylsilyl-cyclohexyl-phthalate.pdf>

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