

tert-Butyldimethylsilyl (E)-hex-3-enyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, (E)-hex-3-enyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C20H30O4Si/c1-7-8-9-12-15-23-18(21)16-13-10-11-14-17(16)19(22)24-25(5,6)
InchiKey:	OJBOKUCZRGHCMX-CMDGGGOBGSA-N
Formula:	C20H30O4Si
SMILES:	CCC=CCCOC(=O)c1cccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	362.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Crippen Method
logp	5.362		Crippen Method
rinpol	2240.00		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=U373629&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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