

(E)-But-2-enyl tert-butyldimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, (E)-but-2-enyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C18H26O4Si/c1-7-8-13-21-16(19)14-11-9-10-12-15(14)17(20)22-23(5,6)18(2,3)
InchiKey:	IONACWMXEPODFB-BQYQJAHWSA-N
Formula:	C18H26O4Si
SMILES:	CC=CCOC(=O)c1ccccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	334.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.21		Crippen Method
logp	4.582		Crippen Method
rinpol	2077.00		NIST Webbook
rinpol	2077.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373508&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/16-493-7/E-But-2-enyl-tert-butyldimethylsilyl-phthalate.pdf>

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