

2,4-Hexadienoic acid, tert-butyldimethylsilyl ester, (E,E)-

Other names:	(tert-Butyldimethyl-silyl) (2E,4E)-hexa-2,4-dienoate
Inchi:	InChI=1S/C12H22O2Si/c1-7-8-9-10-11(13)14-15(5,6)12(2,3)4/h7-10H,1-6H3/b8-7+,10-9-
InchiKey:	RMMQSJCVPYRGHF-XBLVEGMJSA-N
Formula:	C12H22O2Si
SMILES:	CC=CC=CC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	226.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.47		Crippen Method
logp	3.667		Crippen Method
rinpol	1405.00		NIST Webbook
rinpol	1405.00		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=U373157&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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