

tert-Butyldimethylsilyl octyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, octyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C22H36O4Si/c1-7-8-9-10-11-14-17-25-20(23)18-15-12-13-16-19(18)21(24)26-
InchiKey:	KOCCGLNGTGZAAJ-UHFFFAOYSA-N
Formula:	C22H36O4Si
SMILES:	CCCCCCCCOC(=O)c1cccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	392.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.03		Crippen Method
logp	6.366		Crippen Method
rinpol	2448.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373512&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/69-361-5/tert-Butyldimethylsilyl-octyl-phthalate.pdf>

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