

tert-Butyldimethylsilyl 2-ethylhexyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 2-ethylhexyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C22H36O4Si/c1-8-10-13-17(9-2)16-25-20(23)18-14-11-12-15-19(18)21(24)26-
InchiKey:	SMLXDUCFVZQXPD-UHFFFAOYSA-N
Formula:	C22H36O4Si
SMILES:	CCCCC(CC)COC(=O)c1ccccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	392.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.79		Crippen Method
logp	6.222		Crippen Method
rinsol	2351.00		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373621&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
rinsol:	Non-polar retention indices

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<https://www.chemeo.com/cid/49-088-1/tert-Butyldimethylsilyl-2-ethylhexyl-phthalate.pdf>

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