

tert-Butyldimethylsilyl 2-chloroethyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 2-chloroethyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C16H23ClO4Si/c1-16(2,3)22(4,5)21-15(19)13-9-7-6-8-12(13)14(18)20-11-10-1
InchiKey:	IXBQBMPHCRFSDG-UHFFFAOYSA-N
Formula:	C16H23ClO4Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)c1ccccc1C(=O)OCCCl
Mol. weight [g/mol]:	342.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Crippen Method
logp	4.244		Crippen Method
rinpol	2105.00		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=U373509&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/55-475-4/tert-Butyldimethylsilyl-2-chloroethyl-phthalate.pdf>

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