

tert-Butyldimethylsilyl 8-chlorooctyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 8-chlorooctyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C22H35ClO4Si/c1-22(2,3)28(4,5)27-21(25)19-15-11-10-14-18(19)20(24)26-17
InchiKey:	VPMKCWDDCUSVRG-UHFFFAOYSA-N
Formula:	C ₂₂ H ₃₅ ClO ₄ Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)c1cccc1C(=O)OCCCCCCCCCl
Mol. weight [g/mol]:	427.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.18		Crippen Method
logp	6.585		Crippen Method
rinpol	2751.00		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=U373651&Units=SI

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/67-729-9/tert-Butyldimethylsilyl-8-chlorooctyl-phthalate.pdf>

Generated by Cheméo on 2024-05-02 22:48:26.861193202 +0000 UTC m=+16979355.781770514.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.