

tert-Butyldimethylsilyl heptadecyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, heptadecyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C31H54O4Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-26-34-29(32)27-
InchiKey:	CVYVHAOEXXLMCW-UHFFFAOYSA-N
Formula:	C31H54O4Si
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)c1cccc1C(=O)O[Si](C)(C)C(C)C
Mol. weight [g/mol]:	518.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.80		Crippen Method
logp	9.877		Crippen Method
rinpol	3372.00		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=U373707&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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