

sec-Butyl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, sec-butyl trimethylsilyl ester
Inchi:	InChI=1S/C15H22O4Si/c1-6-11(2)18-14(16)12-9-7-8-10-13(12)15(17)19-20(3,4)5/h7-11H
InchiKey:	KDUIPLWLIPEGIJ-UHFFFAOYSA-N
Formula:	C15H22O4Si
SMILES:	CCC(C)OC(=O)c1ccccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	294.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	3.634		Crippen Method
rinpola	1779.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373632&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/25-781-7/sec-Butyl-trimethylsilyl-phthalate.pdf>

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