

Isobutyl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, isobutyl trimethylsilyl ester
Inchi:	InChI=1S/C15H22O4Si/c1-11(2)10-18-14(16)12-8-6-7-9-13(12)15(17)19-20(3,4)5/h6-9,1
InchiKey:	SUKIVXBKIGPRQV-UHFFFAOYSA-N
Formula:	C15H22O4Si
SMILES:	CC(C)COC(=O)c1cccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	294.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.86		Crippen Method
logp	3.491		Crippen Method
rinpol	1787.00		NIST Webbook
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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=U373488&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/49-853-1/Isobutyl-trimethylsilyl-phthalate.pdf>

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