

3-Methylbutan-2-yl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 3-methylbutan-2-yl trimethylsilyl ester
Inchi:	InChI=1S/C16H24O4Si/c1-11(2)12(3)19-15(17)13-9-7-8-10-14(13)16(18)20-21(4,5)6/h7-
InchiKey:	BPKWWSSFHRDXKM-UHFFFAOYSA-N
Formula:	C16H24O4Si
SMILES:	CC(C)C(C)OC(=O)c1ccccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	308.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	3.880		Crippen Method
rinpol	1843.00		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=U373634&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/34-346-0/3-Methylbutan-2-yl-trimethylsilyl-phthalate.pdf>

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