

3-Oxobutan-2-yl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 3-oxobutan-2-yl trimethylsilyl ester
Inchi:	InChI=1S/C15H20O5Si/c1-10(16)11(2)19-14(17)12-8-6-7-9-13(12)15(18)20-21(3,4)5/h6-
InchiKey:	LJQDFCZZNGFXSM-UHFFFAOYSA-N
Formula:	C15H20O5Si
SMILES:	CC(=O)C(C)OC(=O)c1ccccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	308.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	2.813		Crippen Method
rinsol	1896.00		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=U373495&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/48-341-0/3-Oxobutan-2-yl-trimethylsilyl-phthalate.pdf>

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