

Trimethylsilyl 4-oxo-4-(4-phenylphenyl)butanoate

Other names:	Trimethylsilyl 4-biphenyl-4-yl-4-oxobutanate Trimethylsilyl 3-(4-biphenylcarbonyl)propionate Trimethylsilyl 4-(4-Biphenyl)-4-oxobutanate
Inchi:	InChI=1S/C19H22O3Si/c1-23(2,3)22-19(21)14-13-18(20)17-11-9-16(10-12-17)15-7-5-4-6
InchiKey:	DRKJEUWVXOOXIB-UHFFFAOYSA-N
Formula:	C19H22O3Si
SMILES:	C[Si](C)(C)OC(=O)CCC(=O)c1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	326.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	4.695		Crippen Method
rinpol	2592.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U372922&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/66-548-1/Trimethylsilyl-4-oxo-4-4-phenylphenyl-butanoate.pdf>

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