

Butyric acid, 4-phenyl-, trimethylsilyl ester

Other names:	Trimethylsilyl 4-phenylbutanoate Butanoic acid, 4-phenyl, trimethylsilyl ester Benzenebutanoic acid, tms derivative
Inchi:	InChI=1S/C13H20O2Si/c1-16(2,3)15-13(14)11-7-10-12-8-5-4-6-9-12/h4-6,8-9H,7,10-11H
InchiKey:	ZYYPVAODSQWOQR-UHFFFAOYSA-N
Formula:	C13H20O2Si
SMILES:	C[Si](C)(C)OC(=O)CCc1ccccc1
Mol. weight [g/mol]:	236.38
CAS:	21273-16-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.28		Crippen Method
logp	3.387		Crippen Method
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook

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=C21273165&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/15-628-8/Butyric-acid-4-phenyl-trimethylsilyl-ester.pdf>

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