

Phenaceturic acid, N-tert-butyldimethylsilyl-, tert-butyldimethylsilyl ester

Other names:	Phenaceturic acid, 2tbdms derivative
Inchi:	InChI=1S/C22H39NO3Si2/c1-21(2,3)27(7,8)23(19(24)16-18-14-12-11-13-15-18)17-20(25)
InchiKey:	HPJUEPHIRTYPPT-UHFFFAOYSA-N
Formula:	C22H39NO3Si2
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)CN(C(=O)Cc1ccccc1)[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	421.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	5.611		Crippen Method
rinpol	2280.30		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=U333160&Units=SI

Legend

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

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