

Benzeneacetic acid, tert-butyldimethylsilyl ester

Other names:	Phenylacetic acid, TBDMS Phenylacetic acid, tert-butyldimethylsilyl ester Phenylacetic acid, DMTBS tert-Butyl(dimethyl)silyl phenylacetate Benzeneacetic acid, tbdms derivative
Inchi:	InChI=1S/C14H22O2Si/c1-14(2,3)17(4,5)16-13(15)11-12-9-7-6-8-10-12/h6-10H,11H2,1-5
InchiKey:	LISQZGMJTHVNMI-UHFFFAOYSA-N
Formula:	C14H22O2Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)Cc1ccccc1
Mol. weight [g/mol]:	250.41
CAS:	78323-99-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.70		Crippen Method
logp	3.777		Crippen Method
rinpol	1527.00		NIST Webbook
rinpol	1534.70		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1527.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78323996&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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