Benzeneacetic acid, «alpha»-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Othernames:	Acetic acid, phenyl(trimethylsiloxy)-, trimethylsilyl ester
	Mandelic acid (ditms)
	Trimethylsilyl-«alpha»-(trimethylsiloxy)phenylacetae
	andelic acid, di(trimethylsilyl) deriv.
	Trimethylsilyl phenyl[(trimethylsilyl)oxy]acetate
	Mandelic acid, bis-TMS
	Mandelic acid, TMS
	Mandelic acid, di(trimethylsilyl) deriv.
	Mandelic acid, trimethylsilyl ether, trimethylsilyl ester
	DL-Mandelic acid, trimethylsilyl ether, trimethylsilyl ester
	Mandelic acid, 2tms derivative
Inchi:	InChI=1S/C14H24O3Si2/c1-18(2,3)16-13(12-10-8-7-9-11-12)14(15)17-19(4,5)6/h7-11,13
InchiKey:	QGQNCTUAZAEYNK-UHFFFAOYSA-N
Formula:	C14H24O3Si2
SMILES:	C[Si](C)(C)OC(=O)C(O[Si](C)(C)C)c1ccccc1
Mol. weight [g/mol]:	296.51
CAS:	2078-19-5

Physical Properties

Property code	Value	Unit	Source
log10ws	0.70		Crippen Method
logp	3.957		Crippen Method
rinpol	1491.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1468.10		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1468.10		NIST Webbook
rinpol	1491.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2078195&Units=SI

Legend

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