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

Other names:	Phenylpyruvic acid oxime, bis(trimethylsilyl)-
	Oximated phenylpyruvic acid, diTMS
	Phenylpyruvic acid, oxime, bis-TMS
	Phenylpyruvic acid, oxime, di-TMS
	Phenylpyruvic acid oxime, 2tms derivative
Inchi:	InChI=1S/C15H25NO3Si2/c1-20(2,3)18-15(17)14(16-19-21(4,5)6)12-13-10-8-7-9-11-13/h
InchiKey:	NVILHXJLJXJNKN-UHFFFAOYSA-N
Formula:	C15H25NO3Si2
SMILES:	C[Si](C)(C)ON=C(Cc1ccccc1)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	323.53
CAS:	55530-64-8

Physical Properties

Property code	Value	Unit	Source
log10ws	0.59		Crippen Method
logp	3.815		Crippen Method
rinpol	1662.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1662.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55530648&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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