

# Benzenepropanoic acid, «alpha»-[[trimethylsilyloxy]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](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/ci9903071>

# Legend

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

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