

# Benzeneacetic acid, 3,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:

3,4-Dihydroxyphenylacetic acid (tms)  
Trimethylsilyl (3,4-bis[(trimethylsilyl)oxy]phenyl)acetate  
Benzeneacetic acid, 3,4-dihydroxy, tris-TMS  
Homoprotocatechuic acid, tris-TMS  
Phenylacetic acid, 3,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester  
Phenylacetic acid, 3,4-dihydroxy, (3TMS)-  
Benzeneacetic acid, 3,4-dihydroxy, TMS  
Homoprotocatechuic acid, TMS  
Phenylacetic acid, 3,4-dihydroxy, TMS  
3,4-Dihydroxyphenylacetic acid, 3tms derivative

**Inchi:** InChI=1S/C17H32O4Si3/c1-22(2,3)19-15-11-10-14(12-16(15)20-23(4,5)6)13-17(18)21-22

**InchiKey:** RYYDTJQPEUI SHG-UHFFFAOYSA-N

**Formula:** C17H32O4Si3

**SMILES:** C[Si](C)(C)OC(=O)Cc1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1

**Mol. weight [g/mol]:** 384.69

**CAS:** 37148-62-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.54		Crippen Method
logp	5.035		Crippen Method
rinpol	1833.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1827.60		NIST Webbook
rinpol	1833.00		NIST Webbook
rinpol	1827.60		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**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=C37148622&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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