

Trimethylsilyl O,O'-bis(trimethylsilyl)vanilpyruvate

Other names:	Phenylpyruvic acid, 4-hydroxy-3-methoxy, (3TMS) Phenylpyruvic acid, 4-hydroxy-3-methoxy, TMS
Inchi:	InChI=1S/C19H34O5Si3/c1-21-17-13-15(11-12-16(17)22-25(2,3)4)14-18(23-26(5,6)7)19
InchiKey:	GNOWUZOUOHJQLC-JXAWBTAJSA-N
Formula:	C19H34O5Si3
SMILES:	COc1cc(C=C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]:	426.73
CAS:	68595-71-1

Physical Properties

Property code	Value	Unit	Source
log10ws	1.10		Crippen Method
logp	5.479		Crippen Method
rinpol	2165.00		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68595711&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

Latest version available from:

<https://www.chemeo.com/cid/59-916-0/Trimethylsilyl-O-O-bis-trimethylsilyl-vanilpyruvate.pdf>

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