

4-Methoxyphenylpyruvic acid, bis(trimethylsilyl) deriv.

Other names:	4-Methoxyphenylpyruvic acid, di-TMS Phenylpyruvic acid, 4-methoxy, TMS
Inchi:	InChI=1S/C16H26O4Si2/c1-18-14-10-8-13(9-11-14)12-15(19-21(2,3)4)16(17)20-22(5,6)7
InchiKey:	IAKVNQLFHQCXOF-NTCAYCPXSA-N
Formula:	C16H26O4Si2
SMILES:	COc1ccc(C=C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)cc1
Mol. weight [g/mol]:	338.55
CAS:	27750-69-2

Physical Properties

Property code	Value	Unit	Source
log10ws	0.11		Crippen Method
logp	4.266		Crippen Method
rinpol	1953.00		NIST Webbook
rinpol	1953.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27750692&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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