

1,2-Ethanediphosphonic acid, tetra-kis(trimethylsilyl) ester

Other names:	1,2-Ethanediphosphonic acid, tetra-trimethylsilyl; ester 1,2-Ethylenediphosphonic acid, tetra-TMS
Inchi:	InChI=1S/C14H40O6P2Si4/c1-23(2,3)17-21(15,18-24(4,5)6)13-14-22(16,19-25(7,8)9)20
InchiKey:	YOWIFSBY LUTCHQ-UHFFFAOYSA-N
Formula:	C14H40O6P2Si4
SMILES:	C[Si](C)(C)OP(=O)(CCP(=O)(O[Si](C)(C)C)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	478.75

Physical Properties

Property code	Value	Unit	Source
log10ws	1.22		Crippen Method
logp	6.779		Crippen Method
rinpola	1923.00		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=U373477&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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/82-577-1/1-2-Ethanediphosphonic-acid-tetra-kis-rimethylsilyl-ester.pdf>

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