

Phosphonic acid, [2-[bis(trimethylsilyl)amino]ethyl]-, bis(trimethylsilyl) ester

Other names: Phosphoethanolamine, TMS # 3

InChI: InChI=1S/C14H40NO3PSi4/c1-20(2,3)15(21(4,5)6)13-14-19(16,17-22(7,8)9)18-23(10,11

InchiKey: MWAPEOTUZLVKOZ-UHFFFAOYSA-N

Formula: C14H40NO3PSi4

SMILES: C[Si](C)(C)OP(=O)(CCN([Si](C)(C)C)[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]: 413.79

CAS: 53044-44-3

Physical Properties

Property code	Value	Unit	Source
log10ws	3.10		Crippen Method
logp	5.854		Crippen Method
rinpol	1623.00		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=C53044443&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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