Phosphoethanolamine, TMS # 1

Inchi: InChI=1S/C8H24NO4PSi2/c1-15(2,3)12-14(10,11-8-7-9)13-16(4,5)6/h7-9H2,1-6H3
InchiKey: KKFHFRRZHWMAJW-UHFFFAOYSA-N
Formula: C8H24NO4PSi2
SMILES: C[Si](C)(C)OP(=O)(OCCN)O[Si](C)(C)C
Mol. weight [g/mol]: 285.43

Physical Properties

Property code	Value	Unit	Source
log10ws	0.77		Crippen Method
logp	2.773		Crippen Method
rinpol	1293.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R401404&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
rinpol: Non-polar retention indices

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https://www.chemeo.com/cid/64-619-4/Phosphoethanolamine-TMS-1.pdf
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