Phosphoethanolamine, TMS # 2

Inchi: InChI=1S/C11H32NO4PSi3/c1-18(2,3)12-10-11-14-17(13,15-19(4,5)6)16-20(7,8)9/h12H,
InchiKey: SFJKXHNFFRRHCH-UHFFFAOYSA-N
Formula: C11H32NO4PSi3
SMILES: C[Si](C)(C)NCCOP(=O)(O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 357.61

Physical Properties

Property code	Value	Unit	Source
log10ws	1.71		Crippen Method
logp	4.239		Crippen Method
rinpol	1599.00		NIST Webbook
rinpol	1599.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R401419&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices