Pentaerythritol, TMS

Other names: 2,2,8,8-tetramethyl-5,5-bis[[(trimethylsilyl)oxy]methyl]-3,7-dioxa-2,8-disilanonane
Inchi: InChI=1S/C17H44O4Si4/c1-22(2,3)18-13-17(14-19-23(4,5)6,15-20-24(7,8)9)16-21-25(10
InchiKey: DCRQMOJXJXVZFC-UHFFFAOYSA-N
Formula: C17H44O4Si4
SMILES: C[Si](C)(C)OCC(CO[Si](C)(C)C)(CO[Si](C)(C)C)CO[Si](C)(C)C
Mol. weight [g/mol]: 424.87
CAS: 2114-25-2

Physical Properties

Property code	Value	Unit	Source
log10ws	4.75		Crippen Method
logp	5.379		Crippen Method
rinpol	1535.00		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=C2114252&Units=SI

Legend

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