Allitol, TMS

Inchi: InChI=1S/C24H62O6Si6/c1-31(2,3)25-19-21(27-33(7,8)9)23(29-35(13,14)15)24(30-36(16
InchiKey: USBJDBWAPKNPCK-WAPCQROESA-N
Formula: C24H62O6Si6
SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(
Mol. weight [g/mol]: 615.26

Physical Properties

Property code	Value	Unit	Source
log10ws	6.85		Crippen Method
logp	7.570		Crippen Method
rinpol	1988.00		NIST Webbook
rinpol	1988.00		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=R71292&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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