

1,2-Heptacosanediol, di-TMS

Inchi: InChI=1S/C33H72O2Si2/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32-33/s1-33
InchiKey: XQWBSGDMEMMJFY-UHFFFAOYSA-N
Formula: C33H72O2Si2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCC(CO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 557.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.02		Crippen Method
logp	12.440		Crippen Method
rinpol	3230.00		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=R58931&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/71-033-6/1-2-Heptacosanediol-di-TMS.pdf>

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