Nonacosan-1-ol, TMS

Inchi:	InChI=1S/C32H68OSi/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-2
InchiKey:	HVSGKTPMMGDVDY-UHFFFAOYSA-N
Formula:	C32H68OSi
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCO[Si](C)(C)C
Mol. weight [g/mol]:	496.97
CAS:	959236-93-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.36		Crippen Method
logp	12.391		Crippen Method
rinpol	3233.10		NIST Webbook
rinpol	3233.10		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C959236932&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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