palatinitol 1, TMS

Inchi:	InChI=1S/C39H96O11Si9/c1-51(2,3)41-29-31-34(46-55(13,14)15)37(49-58(22,23)24)38(
InchiKey:	MHRRBIHJBBEMLC-FTRYFTPOSA-N
Formula:	C39H96O11Si9
SMILES:	C[Si](C)(C)OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(COC1OC(CO[Si](C)(C)C
Mol. weight [g/mol]:	993.94

Physical Properties

Property code	Value	Unit	Source
log10ws	10.04		Crippen Method
logp	10.972		Crippen Method
rinpol	3037.60		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R489028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/33-792-6/palatinitol-1-TMS.pdf

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