«alpha»-Cellobiose TMS

Other names:	«alpha»-D(+)-Cellobiose, TMS
Inchi:	InChI=1S/C36H86O11Si8/c1-48(2,3)37-25-27-29(31(43-51(10,11)12)34(46-54(19,20)21)
InchiKey:	QJZFVYJIGWEKIR-UNVZJPJOSA-N
Formula:	C36H86O11Si8
SMILES:	C[Si](C)(C)OCC1OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1OC1OC(CO[Si](C)
Mol. weight [g/mol]:	919.75

Physical Properties

Property code	Value	Unit	Source
log10ws	8.84		Crippen Method
logp	9.476		Crippen Method
rinpol	2758.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R24510&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/57-099-0/alpha-Cellobiose-TMS.pdf
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