

Trehalose, TMS

Other names:	«alpha», «alpha»-Tregalose, TMS A,A-Trehalose TMS D(+)-Trehalose (Mycose), TMS Trehalose, oxime-TMS TREHALOSE 8TMS
Inchi:	InChI=1S/C36H86O11Si8/c1-48(2,3)37-25-27-29(42-50(7,8)9)31(44-52(13,14)15)33(46-5
InchiKey:	YQFZNYCPHIXROS-NGKVRULWSA-N
Formula:	C36H86O11Si8
SMILES:	C[Si](C)(C)OCC1OC(OC2OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C2O[Si](C)(C)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	2840.00		NIST Webbook
rinpol	2816.00		NIST Webbook
rinpol	2816.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R24695&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/40-314-8/Trehalose-TMS.pdf>

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