

Xylitol, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-

Other names:	Trimethylsilyl ether of xylitol Xylitol, pentakis-O-(trimethylsilyl)- Xylitol (5TMS) Xylitol, pentakis-TMS Xylitol, TMS Xylitol, pentakis(trimethylsilyl) ether Xylitol, 5tms derivative
Inchi:	InChI=1S/C20H52O5Si5/c1-26(2,3)21-16-18(23-28(7,8)9)20(25-30(13,14)15)19(24-29(10,11)12)22-17-14(20,21)3
InchiKey:	SUZLPERYXSOGNY-PMOLBWCYSA-N
Formula:	C20H52O5Si5
SMILES:	C[Si](C)(C)OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	513.05
CAS:	14199-72-5

Physical Properties

Property code	Value	Unit	Source
log10ws	5.78		Crippen Method
logp	6.350		Crippen Method
rinpol	1744.50		NIST Webbook
rinpol	1739.00		NIST Webbook
rinpol	1682.70		NIST Webbook
rinpol	1703.70		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1744.50		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=C14199725&Units=SI

Legend

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

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