

Trimethylsilyl ether of glucitol

Other names:	d-Glucitol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)- Glucitol, hexakis-O-(trimethylsilyl)-, d- 1,2,3,4,5,6-Hexakis-O-(trimethylsilyl)glucitol D-Glucitol, hexakis-TMS Glucitol, hexakis-TMS Sorbitol, hexakis-O-(trimethylsilyl)-ether Sorbitol, (6TMS) Sorbitol, TMS Glucitol, TMS D-Glucitol, TMS D-Sorbitol (Glucitol), TMS D-glucitol, 6tms derivative
Inchi:	InChI=1S/C24H62O6Si6/c1-31(2,3)25-19-21(27-33(7,8)9)23(29-35(13,14)15)24(30-36(16,17)18)32(34,35)36
InchiKey:	USBJDBWAPKNPCK-UEQSERJNSA-N
Formula:	C24H62O6Si6
SMILES:	C[Si](C)(C)OCC(O[Si](C)(C)C)C(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]:	615.26
CAS:	14199-80-5

Physical Properties

Property code	Value	Unit	Source
log10ws	6.85		Crippen Method
logp	7.570		Crippen Method
rinpol	1979.00		NIST Webbook
rinpol	1931.10		NIST Webbook
rinpol	1982.00		NIST Webbook
rinpol	2005.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	1935.10		NIST Webbook
rinpol	1982.00		NIST Webbook
rinpol	1982.00		NIST Webbook
rinpol	1979.00		NIST Webbook
rinpol	1935.10		NIST Webbook
rinpol	1981.00		NIST Webbook
rinpol	2000.10		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C14199805&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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<https://www.chemeo.com/cid/14-101-3/Trimethylsilyl-ether-of-glucitol.pdf>

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