

D-Sorbitol, hexakis(trimethylsilyl) ether

Other names:	Sorbital, TMS
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)22(34-38(19,20)26)O1
InchiKey:	USBJDBWAPKNPCK-UHFFFAOYSA-N
Formula:	C ₂₄ H ₆₂ O ₆ Si ₆
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

Physical Properties

Property code	Value	Unit	Source
log10ws	6.85		Crippen Method
logp	7.570		Crippen Method
rinpol	1988.00		NIST Webbook
rinpol	1919.70		NIST Webbook
rinpol	1919.70		NIST Webbook
rinpol	1988.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380145&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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