

Iditol, 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(32-34(10,11)12)6
InchiKey:	USBJDBWAPKNPCK-LWSSLDFYSA-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

Physical Properties

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

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R74305&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/55-741-8/Iditol-TMS.pdf>

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