

Inositol, isomer # 2, hexakis-TMS

Other names:	Inositol, isomer # 2, TMS
Inchi:	InChI=1S/C24H60O6Si6/c1-31(2,3)25-19-20(26-32(4,5)6)22(28-34(10,11)12)24(30-36(13,14)16)18
InchiKey:	FRTKXRNTVMCAKI-HPEVMFQJSA-N
Formula:	C ₂₄ H ₆₀ O ₆ Si ₆
SMILES:	C[Si](C)(C)OC1C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]:	613.24

Physical Properties

Property code	Value	Unit	Source
log10ws	6.74		Crippen Method
logp	7.321		Crippen Method
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	2000.00		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=R573574&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/67-048-5/Inositol-isomer-2-hexakis-TMS.pdf>

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