

myo-Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-

Other names:

Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-, myo-

myo-Inositol (6TMS)

mio-Inositol, hexakis-TMS

Myoinositol TMS

INOSITOL 6TMS

myo-Inositol, hexakis(trimethylsilyl) ether

Inositol (myo-Inositol), TMS

Myo-inositol, 6tms derivative

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(16,17)18)23(13,14)15

InchiKey:

FRTKXRNTVMCAKI-UHFFFAOYSA-N

Formula:

C₂₄H₆₀O₆Si₆

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

CAS:

2582-79-8

Physical Properties

Property code	Value	Unit	Source
log10ws	6.74		Crippen Method
logp	7.321		Crippen Method
rinpol	2130.00		NIST Webbook
rinpol	2073.70		NIST Webbook
rinpol	2083.70		NIST Webbook
rinpol	2096.00		NIST Webbook
rinpol	2136.00		NIST Webbook
rinpol	2153.00		NIST Webbook
rinpol	2129.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2130.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2582798&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.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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