

3-O-Methylgulonic acid, pentakis-TMS

Inchi:	InChI=1S/C22H54O7Si5/c1-24-20(21(28-33(11,12)13)22(23)29-34(14,15)16)19(27-32(8,
InchiKey:	GABHOMJIRKCOOC-UHFFFAOYSA-N
Formula:	C22H54O7Si5
SMILES:	COC(C(O[Si](C)(C)C)C(=O)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]:	571.09

Physical Properties

Property code	Value	Unit	Source
log10ws	5.97		Crippen Method
logp	5.891		Crippen Method
rinpol	1938.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R101456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.cheméo.com/cid/10-736-3/3-O-Methylgulonic-acid-pentakis-TMS.pdf>

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