

Gulonic acid, TMS

Other names:	Gulonic acid, hexakis-TMS
Inchi:	InChI=1S/C24H60O7Si6/c1-32(2,3)26-19-20(27-33(4,5)6)21(28-34(7,8)9)22(29-35(10,11)12)31(13,14)15(16,17)18
InchiKey:	IVIMVRAMMWQMHHJ-KAOXLYBCSA-N
Formula:	C ₂₄ H ₆₀ O ₇ 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(O[Si](C)(C)C)C(O[Si](C)(C)C)C(=O)O[S
Mol. weight [g/mol]:	629.24

Physical Properties

Property code	Value	Unit	Source
log10ws	7.08		Crippen Method
logp	7.096		Crippen Method
rinpola	2029.00		NIST Webbook
rinpola	1959.20		NIST Webbook
rinpola	2029.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R101807&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/22-112-2/Gulonic-acid-TMS.pdf>

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