

3-Deoxy-erythro-pentarc acid, TMS

Inchi:	InChI=1S/C17H40O6Si4/c1-24(2,3)20-14(16(18)22-26(7,8)9)13-15(21-25(4,5)6)17(19)23
InchiKey:	KJJOKCNZSWRSBI-HUUCEWRRSA-N
Formula:	C17H40O6Si4
SMILES:	C[Si](C)(C)OC(=O)C(CC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	452.84

Physical Properties

Property code	Value	Unit	Source
log10ws	4.73		Crippen Method
logp	4.573		Crippen Method
rinpol	1721.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R101263&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
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/24-753-9/3-Deoxy-erythro-pentarc-acid-TMS.pdf>

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