

3-Deoxy-2-C-hydroxymethyl-erythro-pentanic acid, TMS

Inchi:	InChI=1S/C21H50O7Si5/c1-29(2,3)24-17-21(28-33(13,14)15,20(23)27-32(10,11)12)16-1
InchiKey:	WNEDAUVACAQDIF-NQIIRXRSSA-N
Formula:	C21H50O7Si5
SMILES:	C[Si](C)(C)OCC(CC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	555.04

Physical Properties

Property code	Value	Unit	Source
log10ws	5.92		Crippen Method
logp	5.795		Crippen Method
rinpol	1963.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R101169&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/15-501-8/3-Deoxy-2-C-hydroxymethyl-erythro-pentanic-acid-TMS.pdf>

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