

erythro-Pentonic acid, 3-deoxy-2,4,5-tris-O-(trimethylsilyl)-2-C-[[trimethylsilyl]ester

Other names:

3-Deoxy-2-C-hydroxymethyl-erythro-pentonic acid, pentakis-TMS

Inchi: InChI=1S/C21H52O6Si5/c1-28(2,3)23-17-19(25-30(7,8)9)16-21(27-32(13,14)15,18-24-29

InchiKey: COPXMBFDIHFMMGG-UHFFFAOYSA-N

Formula: C21H52O6Si5

SMILES: C[Si](C)(C)OCC(CC(CO[Si](C)(C)C)(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]: 541.06

CAS: 55517-79-8

Physical Properties

Property code	Value	Unit	Source
log10ws	5.70		Crippen Method
logp	6.268		Crippen Method
rinpol	1931.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55517798&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

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