

Arabino-hexaric acid, 3-deoxy-2,4,5-tris-O-(trimethylsilyl)-, bis(trimethylsilyl) ester

Other names:	16-Bis(trimethylsilyl)-3-deoxy-2,4,5-tris-O-(trimethylsilyl)arabino-hexarate 3-Deoxy-arabino-hexaric acid, pentakis-TMS 3-Deoxy-arabino-hexaric acid, TMS
Inchi:	InChI=1S/C21H50O7Si5/c1-29(2,3)24-17(19(26-31(7,8)9)21(23)28-33(13,14)15)16-18(20)
InchiKey:	ZJKJLJLIOZASHHC-CEXWTWQISA-N
Formula:	C21H50O7Si5
SMILES:	C[Si](C)(C)OC(=O)C(CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	555.04
CAS:	38165-99-0

Physical Properties

Property code	Value	Unit	Source
log10ws	5.81		Crippen Method
logp	5.793		Crippen Method
rinpol	1949.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38165990&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

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