

Arabino-Hexonic acid, 3-deoxy-2,4,5,6-tetrakis-O-(trimethylsilyl)-, trimethylsilyl ester

Other names:	D-Arabino-Hexonic acid, 3-deoxy-2,4,5,6-tetrakis-O-(trimethylsilyl)-, trimethylsilyl ester 3-Deoxy-arabino-hexonic acid, pentakis-TMS 3-Deoxyhexonic acid, 5tms derivative
Inchi:	InChI=1S/C21H52O6Si5/c1-28(2,3)23-17-20(26-31(10,11)12)18(24-29(4,5)6)16-19(25-30)5
InchiKey:	VXOUZNJSOAZDPY-AABGKKOBSA-N
Formula:	C21H52O6Si5
SMILES:	C[Si](C)(C)OCC(O[Si](C)(C)C)C(CC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	541.06
CAS:	55517-66-3

Physical Properties

Property code	Value	Unit	Source
log10ws	5.59		Crippen Method
logp	6.266		Crippen Method
rinpol	1921.00		NIST Webbook
rinpol	1902.00		NIST Webbook
rinpol	1921.00		NIST Webbook
rinpol	1902.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55517663&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

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