«beta»-Allopyranose, TMS

Inchi:	InChI=1S/C21H52O6Si5/c1-28(2,3)22-16-17-18(24-29(4,5)6)19(25-30(7,8)9)20(26-31(10
InchiKey:	PPFHNIVPOLWPCF-UQVNRYHBSA-N
Formula:	C21H52O6Si5
SMILES:	C[Si](C)(C)OCC1OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]:	541.06

Physical Properties

Property code	Value	Unit	Source
log10ws	5.66		Crippen Method
logp	6.075		Crippen Method
rinpol	1879.00		NIST Webbook
rinpol	1879.00		NIST Webbook
ripol	1778.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R52591&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

Latest version available from:
https://www.chemeo.com/cid/32-634-2/beta-Allopyranose-TMS.pdf
Generated by Cheméo on 2024-10-12 08:40:35.102137744 +0000 UTC m=+3303297.739106991.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.