

1-Kestose, TMS

Inchi:	InChI=1S/C51H120O16Si11/c1-68(2,3)53-34-39-42(61-72(13,14)15)45(64-75(22,23)24)4
InchiKey:	SWHJUYJGRRIDPF-DOJLZCONSA-N
Formula:	C51H120O16Si11
SMILES:	C[Si](C)(C)OCC1OC(OC2(COC3(CO[Si](C)(C)C)OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C3O
Mol. weight [g/mol]:	1298.43

Physical Properties

Property code	Value	Unit	Source
log10ws	12.25		Crippen Method
logp	12.881		Crippen Method
rinpol	3360.00		NIST Webbook
rinpol	3360.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R614378&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

Latest version available from:

<https://www.cheméo.com/cid/119-504-0/1-Kestose-TMS.pdf>

Generated by Cheméo on 2024-04-28 11:02:34.030999151 +0000 UTC m=+16591402.951576466.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.