

Sorbitol, 3,6-dimethyl, TMS

Inchi: InChI=1S/C20H50O6Si4/c1-21-15-17(24-28(6,7)8)20(26-30(12,13)14)19(22-2)18(25-29)
InchiKey: ZOIUFZGNKPBEEW-FYQPLNBISA-N
Formula: C20H50O6Si4
SMILES: COCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(OC)C(CO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 498.95

Physical Properties

Property code	Value	Unit	Source
log10ws	4.63		Crippen Method
logp	5.160		Crippen Method
rinpol	1835.00		NIST Webbook
rinpol	1833.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527774&Units=SI>

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.chemeo.com/cid/57-747-0/Sorbitol-3-6-dimethyl-TMS.pdf>

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