

D(+)-Ononitol, TMS

Inchi: InChI=1S/C22H54O6Si5/c1-23-17-18(24-29(2,3)4)20(26-31(8,9)10)22(28-33(14,15)16)2
InchiKey: IKOVQCQLJNHSBD-VMQUQCCTSA-N
Formula: C22H54O6Si5
SMILES: COC1C(O[Si](C)(C)C)C(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]: 555.09

Physical Properties

Property code	Value	Unit	Source
log10ws	5.62		Crippen Method
logp	6.115		Crippen Method
rinpol	2000.00		NIST Webbook
rinpol	2008.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R531956&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/31-852-1/D-Ononitol-TMS.pdf>

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