

Methyl glucuronide, TMS

Inchi: InChI=1S/C17H38O7Si3/c1-19-16(18)14-12(22-25(3,4)5)13(23-26(6,7)8)15(17(20-2)21-10)
InchiKey: YBPUSDOFUOGIOU-UHFFFAOYSA-N
Formula: C17H38O7Si3
SMILES: COC(=O)C1OC(OC)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 438.74

Physical Properties

Property code	Value	Unit	Source
log10ws	3.66		Crippen Method
logp	3.191		Crippen Method
rinpol	1983.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R554637&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/48-865-9/Methyl-glucuronide-TMS.pdf>

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