p-Tolyl-«beta»-D-glucuronide, tris(trimethylsilyl) ether, trimethylsilyl ester

Inchi: InChI=1S/C25H48O7Si4/c1-18-14-16-19(17-15-18)27-25-23(31-35(8,9)10)21(30-34(5,6)

InchiKey: KEYSANSPWMIMAN-UHFFFAOYSA-N

Formula: C25H48O7Si4

SMILES: Cc1ccc(OC2OC(C(=O)O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C2O[Si](C)(C)C)cc1

Mol. weight [g/mol]: 572.99

Physical Properties

Property code	Value	Unit	Source
log10ws	2.45		Crippen Method
logp	6.137		Crippen Method
rinpol	2419.30		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U380159&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices