3-Trimethylsilyloxy-2-methylpyran-4-one

Other names: 3-Hydroxy-2-methyl-pyran-4-one TMS
Inchi: InChI=1S/C9H14O3Si/c1-7-9(12-13(2,3)4)8(10)5-6-11-7/h5-6H,1-4H3
InchiKey: JAMVNVJEEYSRKJ-UHFFFAOYSA-N
Formula: C9H14O3Si
SMILES: Cc1occc(=O)c1O[Si](C)(C)C
Mol. weight [g/mol]: 198.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	2.162		Crippen Method
rinpol	1293.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373047&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices