

o-Vanillin, TMS

Inchi: InChI=1S/C11H16O3Si/c1-13-11-9(8-12)6-5-7-10(11)14-15(2,3)4/h5-8H,1-4H3
InchiKey: GPCGLWKQPXCXY-UHFFFAOYSA-N
Formula: C11H16O3Si
SMILES: COc1c(C=O)cccc1O[Si](C)(C)C
Mol. weight [g/mol]: 224.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.84		Crippen Method
logp	2.721		Crippen Method
rinpol	1496.00		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=R92620&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/11-299-8/o-Vanillin-TMS.pdf>

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