Ethylvanilline, MO TMS

Inchi: InChI=1S/C13H21NO3Si/c1-6-16-13-9-11(10-14-15-2)7-8-12(13)17-18(3,4)5/h7-10H,6H2
InchiKey: XLNPHAALBQSBFA-UVTDQMKNSA-N
Formula: C13H21NO3Si
SMILES: CCOc1cc(C=NOC)ccc1O[Si](C)(C)C
Mol. weight [g/mol]: 267.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.16		Crippen Method
logp	3.279		Crippen Method
rinpol	1675.00		NIST Webbook
rinpol	1675.00		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=R92563&Units=SI

Legend

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