1-mercaptophenyl-2-pentanol, TMS

Inchi: InChI=1S/C14H24OSSi/c1-5-9-13(15-17(2,3)4)12-16-14-10-7-6-8-11-14/h6-8,10-11,13H,
InchiKey: MVVWEQYJELKVBQ-UHFFFAOYSA-N
Formula: C14H24OSSi
SMILES: CCCC(CSc1ccccc1)O[Si](C)(C)C
Mol. weight [g/mol]: 268.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	4.799		Crippen Method
rinpol	1620.00		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=R497064&Units=SI

Legend

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