2-mercaptophenyl-1-pentanol, TMS

Inchi:	InChI=1S/C14H24OSSi/c1-5-9-14(12-15-17(2,3)4)16-13-10-7-6-8-11-13/h6-8,10-11,14H,
InchiKey:	KDIIMBZCPSIYQC-UHFFFAOYSA-N
Formula:	C14H24OSSi
SMILES:	CCCC(CO[Si](C)(C)C)Sc1ccccc1
Mol. weight [g/mol]:	268.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	4.799		Crippen Method
rinpol	1640.00		NIST Webbook
rinpol	1640.00		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=R497079&Units=SI

Legend

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

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