

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/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/29-374-5/2-mercaptophenyl-1-pentanol-TMS.pdf>

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