

2-Thiophenemethanol, «alpha»-methyl, TMS

Inchi: InChI=1S/C9H16OSSi/c1-8(10-12(2,3)4)9-6-5-7-11-9/h5-8H,1-4H3
InchiKey: FPCTYDDKQGBKRK-UHFFFAOYSA-N
Formula: C9H16OSSi
SMILES: CC(O[Si](C)(C)C)c1cccs1
Mol. weight [g/mol]: 200.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Crippen Method
logp	3.661		Crippen Method
rinpol	1160.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R36711&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/59-567-8/2-Thiophenemethanol-alpha-methyl-TMS.pdf>

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