3-Methylbenzenethiol, S-trimethylsilyl-

Other names: 3-Methylbenzenethiol, tms derivative
Inchi: InChI=1S/C10H16SSi/c1-9-6-5-7-10(8-9)11-12(2,3)4/h5-8H,1-4H3
InchiKey: SKKVUXTWPVWKRE-UHFFFAOYSA-N
Formula: C10H16SSi
SMILES: Cc1cccc(S[Si](C)(C)C)c1
Mol. weight [g/mol]: 196.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.58		Crippen Method
logp	3.922		Crippen Method
rinpol	1324.40		NIST Webbook
rinpol	1324.40		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=U353006&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/91-360-1/3-Methylbenzenethiol-S-trimethylsilyl.pdf
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