2,4-Dimethylbenzenethiol, S-(tert-butyldimethylsilyl)-

Other names: 2,4-Dimethylbenzenethiol, tbdms derivative
Inchi: InChI=1S/C14H24SSi/c1-11-8-9-13(12(2)10-11)15-16(6,7)14(3,4)5/h8-10H,1-7H3
InchiKey: AARCDAOQVNCNMA-UHFFFAOYSA-N
Formula: C14H24SSi
SMILES: Cc1ccc(S[Si](C)(C)C(C)(C)C)c(C)c1
Mol. weight [g/mol]: 252.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	5.401		Crippen Method
rinpol	1671.50		NIST Webbook
rinpol	1671.50		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=U353014&Units=SI

Legend

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