

2-Hydroxythiophenol, S-(tert-butyl dimethylsilyl)-, tert-butyl dimethylsilyl ether

Other names:

2-Mercaptothiophenol, 2thiols derivative

Inchi: InChI=1S/C18H34O3Si2/c1-17(2,3)21(7,8)19-15-13-11-12-14-16(15)20-22(9,10)18(4,5)6

InchiKey: NKBQPFBRTJZLCX-UHFFFAOYSA-N

Formula: C18H34OSSi2

SMILES: CC(C)(C)[Si](C)(C)Oc1cccc1S[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 354.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.62		Crippen Method
logp	7.168		Crippen Method
rinpol	1959.20		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U353061&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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