4-Mercaptobenzoic acid, S-(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Other names: 4-Mercaptobenzoic acid, O,S-di(tert.-butyldimethylsilyl)-
Inchi: InChI=1S/C19H34O2SSi2/c1-18(2,3)23(7,8)21-17(20)15-11-13-16(14-12-15)22-24(9,10)
InchiKey: FFSPXKWBPAUYAU-UHFFFAOYSA-N
Formula: C19H34O2SSi2
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccc(S[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]: 382.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	6.946		Crippen Method
rinpol	2303.00		NIST Webbook
rinpol	2308.90		NIST Webbook
rinpol	2303.00		NIST Webbook
rinpol	2308.90		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U352982&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.