

3-Mercaptobenzoic acid, S-(tert-butyl dimethylsilyl)-, tert-butyl dimethylsilyl ester

Other names: 3-Mercaptobenzoic acid, O,S-di(tert-butyl dimethylsilyl)-

Inchi: InChI=1S/C₁₉H₃₄O₂SSi₂/c1-18(2,3)23(7,8)21-17(20)15-12-11-13-16(14-15)22-24(9,10)

InchiKey: WKMWZLNMQYYVJJ-UHFFFAOYSA-N

Formula: C₁₉H₃₄O₂SSi₂

SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cccc(S[Si](C)(C)C(C)(C)C)c1

Mol. weight [g/mol]: 382.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	6.946		Crippen Method
rinpol	2232.00		NIST Webbook
rinpol	2236.40		NIST Webbook
rinpol	2232.00		NIST Webbook
rinpol	2236.40		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=U352986&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/117-714-9/3-Mercaptobenzoic-acid-S-tert-butyl dimethylsilyl-tert-butyl dimethylsilyl-ester>.

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