

3,5-Di-tert-butyl-4-hydroxybenzoic acid, trimethylsilyl ester

Other names: 3,5-Di-tert-butyl-4-hydroxybenzoic acid, tms derivative

Inchi: InChI=1S/C18H30O3Si/c1-17(2,3)13-10-12(16(20)21-22(7,8)9)11-14(15(13)19)18(4,5)6/

InchiKey: BJZSPZOYHFAVJV-UHFFFAOYSA-N

Formula: C18H30O3Si

SMILES: CC(C)(C)c1cc(C(=O)O[Si](C)(C)C)cc(C(C)(C)C)c1O

Mol. weight [g/mol]: 322.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	4.979		Crippen Method
rinpol	1925.50		NIST Webbook

Sources

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U352486&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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