

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

Other names:	3,5-Di-tert-butyl-4-hydroxybenzoic acid, tbdms derivative
Inchi:	InChI=1S/C21H36O3Si/c1-19(2,3)15-12-14(13-16(17(15)22)20(4,5)6)18(23)24-25(10,11)
InchiKey:	KBKIFSSJQAIYIG-UHFFFAOYSA-N
Formula:	C21H36O3Si
SMILES:	CC(C)(C)c1cc(C(=O)O[Si](C)(C)C(C)(C)C)cc(C(C)(C)C)c1O
Mol. weight [g/mol]:	364.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	6.149		Crippen Method
rinsol	2167.40		NIST Webbook
rinsol	2167.40		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352485&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/50-693-7/3-5-Di-tert-butyl-4-hydroxybenzoic-acid-tert-butyldimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-25 06:14:28.696876255 +0000 UTC m=+16314917.617453582.

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