

tert-Butyldimethylsilyl 2-((tert-butyldimethylsilyl)oxy)-4-methylbenzoate

Other names:

50-85-1, BDMS

3-Cresotinic acid, TBDMS

Inchi: InChI=1S/C20H36O3Si2/c1-15-12-13-16(18(21)23-25(10,11)20(5,6)7)17(14-15)22-24(8,9)

InchiKey: KZABARFQHHZEPM-UHFFFAOYSA-N

Formula: C20H36O3Si2

SMILES: Cc1ccc(C(=O)O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C)(C)C)c1

Mol. weight [g/mol]: 380.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.60		Crippen Method
logp	6.541		Crippen Method
rinpol	2042.00		NIST Webbook
rinpol	2042.00		NIST Webbook

Sources

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U385829&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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