1,2-Benzenedicarboxylic acid, bis(tert-butyldimethylsilyl) ester

Other names: Phthalic acid, (2TBDMS)-
1,2-Benzenedicarboxylic acid, bis[(1,1-dimethylethyl)dimethylsilyl] ester
Phthalic acid, TBDMS
Phthalic acid, DMTBS
Phthalic acid, 2tbdms derivative

Inchi: InChI=1S/C20H34O4Si2/c1-19(2,3)25(7,8)23-17(21)15-13-11-12-14-16(15)18(22)24-26(

InchiKey: RUGOPMVYGOPNSG-UHFFFAOYSA-N

Formula: C20H34O4Si2

SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccccc1C(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 394.65

CAS: 104256-00-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	6.011		Crippen Method
rinpol	2137.00		NIST Webbook
rinpol	2139.99		NIST Webbook
rinpol	2143.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104256000&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