3,4-Dihydroxybenzylamine, N-isoBOC, O-TBDMS

Inchi: InChI=1S/C24H45NO4Si2/c1-18(2)17-27-22(26)25-16-19-13-14-20(28-30(9,10)23(3,4)5)

InchiKey: ADJJDUGHPCMVNR-UHFFFAOYSA-N

Formula: C24H45NO4Si2

SMILES: CC(C)COC(=O)NCc1ccc(O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C)(C)C)c1

Mol. weight [g/mol]: 467.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Crippen Method
logp	7.337		Crippen Method
rinpol	2890.00		NIST Webbook
rinpol	2890.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R392360&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices