3-Aminobenzoic acid, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C16H25NO4Si/c1-7-20-15(19)17-13-10-8-9-12(11-13)14(18)21-22(5,6)16(2,3)4

InchiKey: DCLMALOQBUTRFX-UHFFFAOYSA-N

Formula: C16H25NO4Si

SMILES: CCOC(=O)Nc1cccc(C(=O)O[Si](C)(C)C(C)(C)C)c1

Mol. weight [g/mol]: 323.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	4.417		Crippen Method
rinpol	2216.00		NIST Webbook
rinpol	2216.00		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R563354&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices