3-Aminosalicylic acid, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C22H39NO5Si2/c1-12-26-20(25)23-17-15-13-14-16(18(17)27-29(8,9)21(2,3)4)

InchiKey: QQPMBULQPJLFFO-UHFFFAOYSA-N

Formula: C22H39NO5Si2

SMILES: CCOC(=O)Nc1cccc(C(=O)O[Si](C)(C)C(C)(C)C)c1O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 453.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	6.801		Crippen Method
rinpol	2528.00		NIST Webbook
rinpol	2528.00		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=R563369&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices