tert-Butyl(dimethyl)silyl 4-(2-aminophenyl)-2-pyrrol[tert-butyl(dimethyl)sily

Other names: tert-Butyl(dimethyl)silyl 4-(2-aminophenyl)-2-([tert-butyl(dimethyl)silyl]amino)-4-oxobutanoate
tert-Butyl(dimethyl)silyl 4-(2-aminophenyl)-2-{[tert-butyl(dimethyl)silyl]amino}-4-oxobutanoate
Kynurenine, 2tbdms derivative

Inchi: InChI=1S/C22H40N2O3Si2/c1-21(2,3)28(7,8)24-18(20(26)27-29(9,10)22(4,5)6)15-19(25)

InchiKey: LCPSUDBMQHCTBI-UHFFFAOYSA-N

Formula: C22H40N2O3Si2

SMILES: CC(C)(C)[Si](C)(C)NC(CC(=O)c1ccccc1N)C(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 436.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.89		Crippen Method
logp	5.353		Crippen Method
rinpol	2599.40		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U332752&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