l-Kynurenine, trimethylsilyl ester

Other names: L-kynurenine, tms derivative
Inchi: InChI=1S/C13H20N2O3Si/c1-19(2,3)18-13(17)11(15)8-12(16)9-6-4-5-7-10(9)14/h4-7,11H
InchiKey: VINGZKBHNPYVCU-UHFFFAOYSA-N
Formula: C13H20N2O3Si
SMILES: C[Si](C)(C)OC(=O)C(N)CC(=O)c1ccccc1N
Mol. weight [g/mol]: 280.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.32		Crippen Method
logp	1.547		Crippen Method
rinpol	2097.40		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=U333749&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices