

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:	<chem>C[Si](C)(C)OC(=O)C(N)CC(=O)c1ccccc1N</chem>
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

Latest version available from:

<https://www.chemeo.com/cid/55-377-3/l-Kynurenine-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-05-03 07:17:27.608440909 +0000 UTC m=+17009896.529018225.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.