

Kynurenine, TMS

Inchi: InChI=1S/C22H44N2O3Si4/c1-28(2,3)23-19-16-14-13-15-18(19)21(26-30(7,8)9)17-20(24)
InchiKey: BKICAIFXCAVFFC-FXBPSFAMSA-N
Formula: C22H44N2O3Si4
SMILES: C[Si](C)(C)Nc1cccc1C(=CC(N[Si](C)(C)C)C(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 496.94

Physical Properties

Property code	Value	Unit	Source
log10ws	2.30		Crippen Method
logp	6.297		Crippen Method
rinpol	2186.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R5255&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/84-408-6/Kynurenine-TMS.pdf>

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