

Tryptophan, 5-methoxy, TMS

Inchi: InChI=1S/C21H38N2O3Si3/c1-25-17-11-12-20-18(14-17)16(15-23(20)28(5,6)7)13-19(22)
InchiKey: WWWSWIROBXFOFS-UHFFFAOYSA-N
Formula: C21H38N2O3Si3
SMILES: COc1ccc2c(c1)c(CC(N[Si](C)(C)C)C(=O)O[Si](C)(C)C)cn2[Si](C)(C)C
Mol. weight [g/mol]: 450.79

Physical Properties

Property code	Value	Unit	Source
log10ws	0.27		Crippen Method
logp	5.047		Crippen Method
rinpol	2390.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529196&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/51-801-5/Tryptophan-5-methoxy-TMS.pdf>

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