

Tryptophan, N-acetyl-5-methoxy, TMS

Inchi: InChI=1S/C20H32N2O4Si2/c1-14(23)21-18(20(24)26-28(6,7)8)11-15-13-22(27(3,4)5)19-
InchiKey: SZMJZKVEUQULNK-UHFFFAOYSA-N
Formula: C20H32N2O4Si2
SMILES: COc1ccc2c(c1)c(CC(NC(C)=O)C(=O)O[Si](C)(C)C)cn2[Si](C)(C)C
Mol. weight [g/mol]: 420.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.04		Crippen Method
logp	3.758		Crippen Method
rinpol	2525.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529205&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/68-071-8/Tryptophan-N-acetyl-5-methoxy-TMS.pdf>

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