

N-Acetyl tyrosine TMS

Other names:	N-acetyltyrosine, triTMS N-acetyltyrosine, 3tms derivative
Inchi:	InChI=1S/C20H37NO4Si3/c1-16(22)21(26(2,3)4)19(20(23)25-28(8,9)10)15-17-11-13-18(
InchiKey:	VOOJHLDVEYVNJS-UHFFFAOYSA-N
Formula:	C20H37NO4Si3
SMILES:	CC(=O)N(C(Cc1ccc(O[Si](C)(C)C)cc1)C(=O)O[Si](C)(C)C)[Si](C)(C)C
Mol. weight [g/mol]:	439.77

Physical Properties

Property code	Value	Unit	Source
log10ws	1.53		Crippen Method
logp	4.873		Crippen Method
rinpol	2119.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U141309&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/13-712-6/N-Acetyl-tyrosine-TMS.pdf>

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