

L-Tyrosine, N,O-bis(trimethylsilyl)-3-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:

Dopa, (4TMS)

Levodopa, N,O,O,O-tetrakis-TMS

LEVODOPA,N,O,O,O-TMS

Dopa, TMS

3-Hydroxy-l-tyrosine, 4tms derivative

Inchi:	InChI=1S/C21H43NO4Si4/c1-27(2,3)22-18(21(23)26-30(10,11)12)15-17-13-14-19(24-28)
InchiKey:	SSTPUELEMUKSOG-SFHVURJKSA-N
Formula:	C21H43NO4Si4
SMILES:	<chem>C[Si](C)(C)NC(Cc1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1)C(=O)O[Si](C)(C)C</chem>
Mol. weight [g/mol]:	485.91
CAS:	55638-45-4

Physical Properties

Property code	Value	Unit	Source
log10ws	2.51		Crippen Method
logp	5.828		Crippen Method
rinpol	2124.00		NIST Webbook
rinpol	2081.40		NIST Webbook
rinpol	2124.00		NIST Webbook
rinpol	2081.40		NIST Webbook

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=C55638454&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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