

3-Iodo-L-tyrosine, N,O-bis(trimethylsilyl)-, trimethylsilyl ester

Other names:	3-Iodo-L-tyrosine, 3tms derivative
Inchi:	InChI=1S/C18H34INO3Si3/c1-24(2,3)20-16(18(21)23-26(7,8)9)13-14-10-11-17(15(19)12
InchiKey:	FMANXQITCFUTIG-UHFFFAOYSA-N
Formula:	C18H34INO3Si3
SMILES:	C[Si](C)(C)NC(Cc1ccc(O[Si](C)(C)C)c(I)c1)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	523.63

Physical Properties

Property code	Value	Unit	Source
log10ws	0.37		Crippen Method
logp	5.219		Crippen Method
rinpol	2242.10		NIST Webbook
rinpol	2242.10		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333512&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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