

5-Hydroxytryptophan, ethoxycarbonylated, TBDMS # 1

Inchi:	InChI=1S/C26H44N2O5Si2/c1-12-31-24(30)28-22(23(29)33-35(10,11)26(5,6)7)15-18-17
InchiKey:	NPVHCWHHMBWIAR-UHFFFAOYSA-N
Formula:	C26H44N2O5Si2
SMILES:	CCOC(=O)NC(Cc1c[nH]c2ccc(O[Si](C)(C)C(C)(C)C)cc12)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	520.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	6.276		Crippen Method
rinpol	3206.00		NIST Webbook
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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=R563849&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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<https://www.chemeo.com/cid/116-127-2/5-Hydroxytryptophan-ethoxycarbonylated-TBDMS-1.pdf>

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