

5-Methoxytryptophan, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C24H36N2O7Si/c1-9-31-22(28)25-19(21(27)33-34(7,8)24(3,4)5)13-16-15-26(2)
InchiKey: LGOGGQXPYBKPSV-UHFFFAOYSA-N
Formula: C24H36N2O7Si
SMILES: CCOC(=O)NC(Cc1cn(C(=O)OCC)c2ccc(OC)cc12)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 492.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.57		Crippen Method
logp	4.860		Crippen Method
rinpol	2929.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R563869&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/37-592-4/5-Methoxytryptophan-ethoxycarbonylated-TBDMS.pdf>

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