

5-Hydroxytryptophan, ethoxycarbonylated, TBDMS # 2

Inchi: InChI=1S/C29H48N2O7Si2/c1-13-35-26(33)30-23(25(32)38-40(11,12)29(6,7)8)17-20-19
InchiKey: MOLAGHPXOIRTBN-UHFFFAOYSA-N
Formula: C29H48N2O7Si2
SMILES: CCOC(=O)NC(Cc1cn(C(=O)OCC)c2ccc(O[Si](C)(C)C(C)(C)C)cc12)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 592.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.71		Crippen Method
logp	7.235		Crippen Method
rinpol	3250.00		NIST Webbook
rinpol	3250.00		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=R563854&Units=SI>

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/122-245-4/5-Hydroxytryptophan-ethoxycarbonylated-TBDMS-2.pdf>

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