

Tryptophan, 5-hydroxy, TMS

Inchi: InChI=1S/C20H36N2O3Si3/c1-26(2,3)22-19(20(23)25-28(7,8)9)12-15-14-21-18-11-10-16
InchiKey: KAQXTWLBAQQBBY-UHFFFAOYSA-N
Formula: C20H36N2O3Si3
SMILES: C[Si](C)(C)NC(Cc1c[nH]c2ccc(O[Si](C)(C)C)cc12)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 436.77
CAS: 56272-77-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.50		Crippen Method
logp	4.613		Crippen Method
rinpol	2451.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C56272776&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/22-616-3/Tryptophan-5-hydroxy-TMS.pdf>

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