

meta-Fluorotyrosine, tris-TMS

Inchi: InChI=1S/C18H34FNO3Si3/c1-24(2,3)20-16(18(21)23-26(7,8)9)13-14-10-11-17(15(19)12)
InchiKey: FPPLWUBSSUMWFJ-UHFFFAOYSA-N
Formula: C18H34FNO3Si3
SMILES: C[Si](C)(C)NC(Cc1ccc(O[Si](C)(C)C)c(F)c1)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 415.72

Physical Properties

Property code	Value	Unit	Source
log10ws	1.19		Crippen Method
logp	4.753		Crippen Method
rinpol	1945.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R493057&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/45-381-9/meta-Fluorotyrosine-tris-TMS.pdf>

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