Valine-glutamine-tryptophan-leucine, N(«alpha»,«epsilon»)-trifluoroacetyl-N-O-permeth derivative

Inchi: InChI=1S/C38H52F6N6O8/c1-21(2)18-28(34(55)58-11)48(8)32(53)27(19-23-20-45(5)25-
InchiKey: NCFZVNIXEYBEPL-UHFFFAOYSA-N
Formula: C38H52F6N6O8
SMILES: COC(=O)C(CC(C)C)N(C)C(=O)C(Cc1cn(C)c2ccccc12)N(C)C(=O)C(CCC(=O)N(C)C(=O)
Mol. weight [g/mol]: 834.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.32		Crippen Method
logp	3.794		Crippen Method
mcvol	594.720	ml/mol	McGowan Method
rinpol	4282.00		NIST Webbook
rinpol	4363.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R248832&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.