Tryptophan-leucine-methionine,N(«alpha»,«epsilo derivative

Inchi: InChI=1S/C29H41F3N4O5S/c1-18(2)15-23(25(37)34(4)22(13-14-42-8)27(39)41-7)35(5)2
InchiKey: HEHKKIVIOCVLIT-UHFFFAOYSA-N
Formula: C29H41F3N4O5S
SMILES: COC(=O)C(CCSC)N(C)C(=O)C(CC(C)C)N(C)C(=O)C(Cc1cn(C)c2ccccc12)N(C)C(=O)C(
Mol. weight [g/mol]: 614.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.44		Crippen Method
logp	3.736		Crippen Method
mcvol	454.280	ml/mol	McGowan Method
rinpol	3420.00		NIST Webbook
rinpol	3519.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R248807&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.