

Tryptophan-leucine, N(«alpha»,«epsilon»)-trifluoroacetyl-N-O-permeth derivative

InChI: InChI=1S/C23H30F3N3O4/c1-14(2)11-19(21(31)33-6)28(4)20(30)18(29(5)22(32)23(24,2
InChIKey: CNUJMBUFBUAVRY-UHFFFAOYSA-N
Formula: C23H30F3N3O4
SMILES: COC(=O)C(CC(C)C)N(C)C(=O)C(Cc1cn(C)c2ccccc12)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 469.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.59		Crippen Method
logp	3.156		Crippen Method
mcvol	341.840	ml/mol	McGowan Method
rinpol	2560.00		NIST Webbook
rinpol	2630.00		NIST Webbook
rinpol	2560.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R248812&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

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