tryptophan, trifluoroacetyl-isopropyl ester

Inchi: InChI=1S/C18H16F6N2O4/c1-9(2)30-14(27)12(25-15(28)17(19,20)21)7-10-8-26(16(29)1
InchiKey: YPZNKHFNKALGBY-UHFFFAOYSA-N
Formula: C18H16F6N2O4
SMILES: CC(C)OC(=O)C(Cc1cn(C(=O)C(F)(F)F)c2ccccc12)NC(=O)C(F)(F)F
Mol. weight [g/mol]: 438.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.09		Crippen Method
logp	3.385		Crippen Method
mcvol	266.720	ml/mol	McGowan Method
rinpol	1994.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R268014&Units=SI
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

Legend

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