

Gly-Pro, butyl ester, TFA

Inchi: InChI=1S/C13H19F3N2O4/c1-2-3-7-22-10(19)8-17-11(20)9-5-4-6-18(9)12(21)13(14,15)1
InchiKey: DMNCGYCOMGMHAA-UHFFFAOYSA-N
Formula: C13H19F3N2O4
SMILES: CCCCOC(=O)CN=C(O)C1CCCN1C(=O)C(F)(F)F
Mol. weight [g/mol]: 324.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	1.840		Crippen Method
mcvol	219.020	ml/mol	McGowan Method
rinpol	1931.00		NIST Webbook
rinpol	1931.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R31985&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/83-151-2/Gly-Pro-butyl-ester-TFA.pdf>

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