Glycine, n-benzyl-n-[6-chloro-5-(2,2,2-trifluoro-n-methylace ethyl ester

Inchi: InChI=1S/C18H18ClF3N4O3/c1-3-29-13(27)10-26(9-12-7-5-4-6-8-12)16-14(15(19)23-11-
InchiKey: YSGQVYKCVJVNBT-UHFFFAOYSA-N
Formula: C18H18ClF3N4O3
SMILES: CCOC(=O)CN(Cc1ccccc1)c1ncnc(Cl)c1N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 430.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	3.225		Crippen Method
mcvol	283.440	ml/mol	McGowan Method

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=B6008441&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume