Triazole-4-carboxylic acid, 1,2,3-, 5-phenylacetamido-

Inchi: InChI=1S/C11H10N4O3/c16-8(6-7-4-2-1-3-5-7)12-10-9(11(17)18)13-15-14-10/h1-5H,6H2

InchiKey: DYRMRYMSPPBFET-UHFFFAOYSA-N

Formula: C11H10N4O3

SMILES: O=C(Cc1ccccc1)Nc1[nH]nnc1C(=O)O

Mol. weight [g/mol]: 246.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.10		Crippen Method
logp	0.202		Crippen Method
mcvol	171.560	ml/mol	McGowan Method

Sources

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=B6008687&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume