Triazolyl-5-carboxamide, 4-phenylamino-

Inchi: InChI=1S/C9H9N5O/c10-8(15)7-9(13-14-12-7)11-6-4-2-1-3-5-6/h1-5H,(H2,10,15)(H2,11,

InchiKey: XJRYKKQIVAFMND-UHFFFAOYSA-N

Formula: C9H9N5O

SMILES: NC(=O)c1[nH]nnc1Nc1ccccc1

Mol. weight [g/mol]: 203.20

CAS: 103754-03-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	0.165		Crippen Method
mcvol	145.920	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103754036&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