

# Triazolyl-5-carboxamide, 4-phenylamino-

<b>Inchi:</b>	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,
<b>InchiKey:</b>	XJRYKKQIVAFMND-UHFFFAOYSA-N
<b>Formula:</b>	C9H9N5O
<b>SMILES:</b>	NC(=O)c1[nH]nnc1Nc1ccccc1
<b>Mol. weight [g/mol]:</b>	203.20
<b>CAS:</b>	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

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C103754036&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C103754036&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/45-531-2/Triazolyl-5-carboxamide-4-phenylamino.pdf>

Generated by Cheméo on 2024-07-18 19:16:08.182424803 +0000 UTC m=+20037.429530149.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.