

# 4-Methyl-2-phenyl-2H-1,2,3-triazole-5-carboxylic acid

Other names:	4-Methyl-2-phenyl-1,2,3-triazole-5-carboxylic acid
Inchi:	InChI=1S/C10H9N3O2/c1-7-9(10(14)15)12-13(11-7)8-5-3-2-4-6-8/h2-6H,1H3,(H,14,15)
InchiKey:	GQYQHAGPALBYDO-UHFFFAOYSA-N
Formula:	C10H9N3O2
SMILES:	Cc1nn(-c2ccccc2)nc1C(=O)O
Mol. weight [g/mol]:	203.20
CAS:	22300-56-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.19		Crippen Method
logp	1.274		Crippen Method
mcvol	145.920	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C22300567&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22300567&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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