

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:	DYRMRYMSPPFET-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/ci9903071

Legend

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

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