

4-Methyl-2-phenyl-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:	<chem>Cc1nn(-c2ccccc2)nc1C(=O)O</chem>
Mol. weight [g/mol]:	203.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.16		Cheméo Relay (1.0)
logp	1.274		Crippen Method
mcvol	145.920	ml/mol	McGowan Method
tb	614.79	K	Cheméo Relay (1.0)
tf	449.05	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22300567&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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