

5-Methyl-1-phenylpyrazole-4-carboxylic acid

Inchi:	InChI=1S/C11H10N2O2/c1-8-10(11(14)15)7-12-13(8)9-5-3-2-4-6-9/h2-7H,1H3,(H,14,15)
InchiKey:	USSMIQWDLWJQDQ-UHFFFAOYSA-N
Formula:	C11H10N2O2
SMILES:	Cc1c(C(=O)O)cnn1-c1ccccc1
Mol. weight [g/mol]:	202.21
CAS:	91138-00-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	1.879		Crippen Method
mcvol	150.030	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=C91138000&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

Latest version available from:

<https://www.chemeo.com/cid/124-033-7/5-Methyl-1-phenylpyrazole-4-carboxylic-acid.pdf>

Generated by Cheméo on 2025-12-25 01:08:59.9320425 +0000 UTC m=+6373137.462083154.

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