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/ci990307l

Legend

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