5-Amino-1-phenylpyrazole-4-carboxamide

Inchi: InChI=1S/C10H10N4O/c11-9-8(10(12)15)6-13-14(9)7-4-2-1-3-5-7/h1-6H,11H2,(H2,12,15

InchiKey: UBKSUPKIDNXMMC-UHFFFAOYSA-N

Formula: C10H10N4O

SMILES: NC(=O)c1cnn(-c2ccccc2)c1N

Mol. weight [g/mol]: 202.21

CAS: 50427-77-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	0.553		Crippen Method
mcvol	150.030	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C50427775&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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