

Imidazole-4-carboxamide, 5-amino-1-cyclopentyl-

Inchi:	InChI=1S/C9H14N4O/c10-8-7(9(11)14)12-5-13(8)6-3-1-2-4-6/h5-6H,1-4,10H2,(H2,11,14)
InchiKey:	ZPQLACOBQASMU-UHFFFAOYSA-N
Formula:	C9H14N4O
SMILES:	NC(=O)c1ncn(C2CCCC2)c1N
Mol. weight [g/mol]:	194.23
CAS:	37642-55-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	0.679		Crippen Method
mcvol	148.840	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=C37642550&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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