

2-Amino-4-p-nitrophenyl oxazole

Inchi:	InChI=1S/C9H7N3O3/c10-9-11-8(5-15-9)6-1-3-7(4-2-6)12(13)14/h1-5H,(H2,10,11)
InchiKey:	OZYUAUHAEUXMQP-UHFFFAOYSA-N
Formula:	C9H7N3O3
SMILES:	<chem>Nc1nc(-c2ccc([N+](=O)[O-])cc2)co1</chem>
Mol. weight [g/mol]:	205.17
CAS:	68101-31-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.86		Crippen Method
logp	1.832		Crippen Method
mcvol	137.700	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C68101315&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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