2-Amino-4-phenyl oxazole

Inchi:	InChI=1S/C9H8N2O/c10-9-11-8(6-12-9)7-4-2-1-3-5-7/h1-6H,(H2,10,11)
InchiKey:	FXRWCCOADRNYMB-UHFFFAOYSA-N
Formula:	C9H8N2O
SMILES:	Nc1nc(-c2ccccc2)co1
Mol. weight [g/mol]:	160.17
CAS:	33119-65-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.21		Crippen Method
logp	1.924		Crippen Method
mcvol	120.280	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=C33119652&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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