

2-Amino-4-(4-nitrophenyl)thiazole

Other names:	Thiazole, 2-amino-4-(p-nitrophenyl)- 2-Amino-4-(p-nitrophenyl)thiazole 2-Thiazolamine, 4-(4-nitrophenyl)- 4-(4-Nitro-phenyl)-thiazol-2-ylamine
Inchi:	InChI=1S/C9H7N3O2S/c10-9-11-8(5-15-9)6-1-3-7(4-2-6)12(13)14/h1-5H,(H2,10,11)
InchiKey:	RIKJWJIWXCUKQV-UHFFFAOYSA-N
Formula:	C9H7N3O2S
SMILES:	<chem>Nc1nc(-c2ccc([N+](=O)[O-])cc2)cs1</chem>
Mol. weight [g/mol]:	221.24
CAS:	2104-09-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Crippen Method
logp	2.300		Crippen Method
mcvol	148.180	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=C2104098&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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