4-(P-NITROPHENYL)-2-THIAZOLAMINE

Other names:	2-Amino-4-(p-nitrophenyl)thiazole
	2-Thiazolamine, 4-(4-nitrophenyl)-
	4-(4-Nitro-phenyl)-thiazol-2-ylamine
	Thiazole, 2-amino-4-(p-nitrophenyl)-
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:	Nc1nc(-c2ccc([N+](=O)[O-])cc2)cs1
Mol. weight [g/mol]:	221.24

Physical Properties

Property code	Value	Unit	Source
hf	203.17	kJ/mol	Cheméo Relay (1.0)
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-3.91		Cheméo Relay (1.0)
logp	2.300		Crippen Method
mcvol	148.180	ml/mol	McGowan Method
tf	487.04	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2104098&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point