2-AMINO-5-NITROPYRIMIDINE

Other names:	2-Pyrimidinamine, 5-nitro-
	5-nitropyrimidin-2-amine
Inchi:	InChI=1S/C4H4N4O2/c5-4-6-1-3(2-7-4)8(9)10/h1-2H,(H2,5,6,7)
InchiKey:	SSHFCFRJYJIJDV-UHFFFAOYSA-N
Formula:	C4H4N4O2
SMILES:	Nc1ncc([N+](=O)[O-])cn1
Mol. weight [g/mol]:	140.10

Physical Properties

Property code	Value	Unit	Source
hf	141.01	kJ/mol	Cheméo Relay (1.0)
ie	9.55	eV	Cheméo Relay (1.0)
log10ws	-1.51		Cheméo Relay (1.0)
logp	-0.033		Crippen Method
mcvol	90.820	ml/mol	McGowan Method
tb	544.05	K	Cheméo Relay (1.0)
tf	486.93	K	Cheméo Relay (1.0)

Sources

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=C3073776&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point