5-Nitroaminotetrazole

Inchi: InChI=1S/CH2N6O2/c8-7(9)4-1-2-5-6-3-1/h(H2,2,3,4,5,6)
InchiKey: HURPOIVZCDCEEE-UHFFFAOYSA-N
Formula: CH2N6O2
SMILES: O=[N+]([O-])Nc1nnn[nH]1
Mol. weight [g/mol]: 130.07
CAS: 18588-16-4

Physical Properties

Property code	Value	Unit	Source
chs	-931.40	kJ/mol	NIST Webbook
hf	252.00	kJ/mol	NIST Webbook
log10ws	-0.65		Crippen Method
logp	-1.679		Crippen Method
mcvol	72.810	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=C18588164&Units=SI

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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