N-Nitro-1H-1,2,4-triazol-3-amine

Other names:	1H-1,2,4-Triazol-3-amine, N-nitro- 3-Nitroamino-1,2,4-triazole
Inchi:	InChI=1S/C2H3N5O2/c8-7(9)6-2-3-1-4-5-2/h1H,(H2,3,4,5,6)
InchiKey:	JKMRKVRTECEDPV-UHFFFAOYSA-N
Formula:	C2H3N5O2
SMILES:	O=[N+]([O-])Nc1nc[nH]n1
Mol. weight [g/mol]:	129.08
CAS:	34815-01-5

Physical Properties

Property code	Value	Unit	Source
chs	-1328.20 ± 4.20	kJ/mol	NIST Webbook
hfs	112.40 ± 4.20	kJ/mol	NIST Webbook
log10ws	-0.89		Crippen Method
logp	-1.074		Crippen Method
mcvol	76.920	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=C34815015&Units=SI

Legend

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