

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/ci9903071>
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

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