5-Methyl-N-nitro-1H-1,2,4-triazol-3-amine

Other names:	1H-1,2,4-Triazol-3-amine, 5-methyl-N-nitro-
	3-Methyl-5-nitroamino-1,2,4-triazone
	3-Methyl-5-nitroamino-1,2,4-triazole
Inchi:	InChI=1S/C3H5N5O2/c1-2-4-3(6-5-2)7-8(9)10/h1H3,(H2,4,5,6,7)
InchiKey:	AKRHSQIJWHJWPC-UHFFFAOYSA-N
Formula:	C3H5N5O2
SMILES:	Cc1n[nH]c(N[N+](=O)[O-])n1
Mol. weight [g/mol]:	143.10
CAS:	42216-41-1

Physical Properties

Property code	Value	Unit	Source
chs	-1948.40 ± 1.60	kJ/mol	NIST Webbook
hfs	53.20 ± 1.60	kJ/mol	NIST Webbook
log10ws	-1.36		Crippen Method
logp	-0.765		Crippen Method
mcvol	91.010	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=C42216411&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