3-METHYL-5-NITROAMINO-1,2,4-TRIAZOLE

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]: 143.11

Physical Properties

Property code	Value	Unit	Source
chs	-1948.40 ± 1.60	kJ/mol	NIST Webbook
hf	123.94	kJ/mol	Cheméo Relay (1.0)
hfs	53.20 ± 1.60	kJ/mol	NIST Webbook
logp	-0.765		Crippen Method
mcvol	91.010	ml/mol	McGowan Method
tb	542.98	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42216411&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature