

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/ci990307I>

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

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