

1-Amino-3-nitroguanidine

Other names: N-nitrocarbazamidine.

InChI: InChI=1S/CH5N5O2/c2-1(4-3)5-6(7)8/h3H2,(H3,2,4,5)

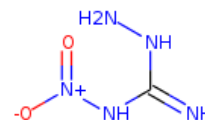
InChI Key: LWPLPMSGDZDOLW-UHFFFAOYSA-N

Formula: CH5N5O2

SMILES: N=C(NN)N[N+](=O)[O-]

Molecular Weight: 119.08

CAS: 18264-75-0



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	441.92	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	264.33	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	70.00	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	-1.83		Crippen Method
T_{boil}	631.33	K	Joback Method
T_{fus}	484.65 ± 2.50	K	NIST Webbook

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	195.04	J/mol×K	631.33	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/CH5N5O2/c2-1\(4-3\)5-6\(7\)8/h3H2,\(H3,2,4,5\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/CH5N5O2/c2-1(4-3)5-6(7)8/h3H2,(H3,2,4,5))

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{oct/wat}$: Octanol/Water partition coefficient .

T_{boil} : Normal Boiling Point Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

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