

Guanidine, nitro-

Other names:	Guanidine, nitro- «alpha»-Nitroguanidine «beta»-Nitroguanidine N''-Nitroguanidine Picrite 1-Nitroguanidine Guanidine, 1-nitro- Guanidine, 1-nitro- (wet) Nitroguanidine, wet N1-Nitroguanidine Picrite (the explosive) 2-Nitroguanidine Guanidine, N-nitro- NSC 41036
Inchi:	InChI=1S/CH4N4O2/c2-1(3)4-5(6)7/h(H4,2,3,4)
InchiKey:	IDCPFAYURAQKDZ-UHFFFAOYSA-N
Formula:	CH4N4O2
SMILES:	NC(N)=N[N+](=O)[O-]
Mol. weight [g/mol]:	104.07

Physical Properties

Property code	Value	Unit	Source
hfs	-86.60 ± 2.50	kJ/mol	NIST Webbook
hfs	-97.90 ± 4.20	kJ/mol	NIST Webbook
hfs	-89.10	kJ/mol	NIST Webbook
hsub	142.70 ± 2.00	kJ/mol	NIST Webbook
logp	-1.548		Crippen Method
mcvol	68.010	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	129.30	J/mol×K	298.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C556887&Units=SI>

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

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

Cheméo Relay (1.0):

Legend

cps: Solid phase heat capacity

hfs: Solid phase enthalpy of formation at standard conditions

hsub: Enthalpy of sublimation at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/49-854-0/Guanidine-nitro.pdf>

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