Acetic acid, (amino(nitroamino)methylene)hydrazide

Other names: 1-Acetamido-3-nitroguanidine
Acetic acid, 2-[imino(nitroamino)methyl]hydrazide
Guanidine, 1-acetamido-3-nitro-
1-Acetamido-2-nitro-guanidine

Inchi: InChI=1S/C3H7N5O3/c1-2(9)5-6-3(4)7-8(10)11/h1H3,(H,5,9)(H3,4,6,7)

InchiKey: UYUTZEZTHPTFOY-UHFFFAOYSA-N

Formula: C3H7N5O3

SMILES: CC(=O)NNC(=N)N[N+](=O)[O-]

Mol. weight [g/mol]: 161.12

CAS: 42216-29-5

Physical Properties

Property code	Value	Unit	Source
chs	-1987.40 ± 5.90	kJ/mol	NIST Webbook
gf	352.78	kJ/mol	Joback Method
hf	130.15	kJ/mol	Joback Method
hfs	-193.60 ± 5.90	kJ/mol	NIST Webbook
hvap	77.00	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	-1.657		Crippen Method
mcvol	107.740	ml/mol	McGowan Method
tb	708.60	K	Joback Method
tf	543.87	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.87	J/mol×K	708.60	Joback Method
cpg	53.15	J/mol×K	100.12	Joback Method
cpg	53.15	J/mol×K	100.12	Joback Method
cpg	53.15	J/mol×K	100.12	Joback Method
cpg	53.15	J/mol×K	100.12	Joback Method
cpg	53.15	J/mol×K	100.12	Joback Method
cpg	53.15	J/mol×K	100.12	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42216295&Units=SI
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
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point