3-Amino-s-triazole

Other names:

1,2,4-triazol-3-amine
1,2,4-triazol-3-ylamine
1,2,4-triazole, 3-amino-
1H-1,2,4-Triazol-3-amine
1H-1,2,4-Triazol-3-ylamine
1H-1,2,4-Triazol-5-amine
1H-1,2,4-Triazole, 3-amino-
1H-1,2,4-Triazole-3-amine
2,3,5,6-Tetraazabicyclo[2.1.1]hex-1-ene
2-Amino-1,3,4-triazole
3-AT
3-Amino-1,2,4-triazol
3-Amino-1,2,4-triazole
3-Amino-1H-1,2,4-triazole
3-Aminotriazole
5-Amino-1,2,4-triazole
5-Amino-1H-1,2,4-triazole
AT
ATA
Amerol
Aminotriazol-spritzpulver
Aminotriazole
Aminotriazole (plant regulator)
Aminotriazole bayer
Amitolamitril
Amitril T.L.
Amitrol
Amitrol 90
Amitrol-T
Amitrole
Amizol
Amizol D
Amizol DP NAU
Amizol F
Azaplant
Azaplant kombi
Azolan
Azole
Campaprim A 1544
Cytrol

	Cytrole
	Diurol 5030
	ENT 25445
	Elmasil
	Emisol
	Emisol 50
	Emisol F
	Fenavar
	Herbidal Total
	Herbizole
	Kleer-Lot
	MSS aminotriazole
	Maxata
	Orga-414
	Radoxone TL
	Ramizol
	Solution concentree T271
	TMG
	Triazolamine
	USAF XR-22
	Vorox
	Vorox AA
	Vorox AS
	Weedar ADS
	Weedar AT
	Weedazin
	Weedazin arginit
	Weedazol
	Weedazol GP2
	Weedazol T
	Weedazol super
	Weedex granulat
	Weedoclor
	s-Triazole, 3-amino-
	x-all Liquid
Inchi:	InChI=1S/C2H4N4/c3-2-4-1-5-6-2/h1H,(H3,3,4,5,6)
InchiKey:	KLSJWNVTNUYHDU-UHFFFAOYSA-N
Formula:	C2H4N4
SMILES:	Nc1nc[nH]n1
Mol. weight [g/mol]:	84.08
CAS:	61-82-5

Physical Properties

Property code	Value	Unit	Source
chs	-1435.50 ± 3.90	kJ/mol	NIST Webbook
hfs	76.80 ± 3.90	kJ/mol	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	0.52		Aqueous Solubility Prediction Method
log10ws	0.52		Estimated Solubility Method
logp	-1.095		Crippen Method
mcvol	59.500	ml/mol	McGowan Method
rinpol	1300.00		NIST Webbook
rinpol	1324.00		NIST Webbook
tf	429.48	K	Aqueous Solubility Prediction Method
tf	429.28 ± 0.20	K	NIST Webbook
tf	428.90 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	21.93	kJ/mol	428.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61825&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solubility determination and thermodynamic modelling of 3-amino-1,2,4-triazole in ten organic solvents from T = 283.15 K to T = 318.15 K and mixing properties of solutions: https://www.doi.org/10.1016/j.jct.2016.09.033

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point