

# 2,4,6-pyrimidinetriamine

Other names:	pyrimidine-2,4,6-triamine
Inchi:	InChI=1S/C4H7N5/c5-2-1-3(6)9-4(7)8-2/h1H,(H6,5,6,7,8,9)
InchiKey:	JTTIOYHBNXDJOD-UHFFFAOYSA-N
Formula:	C4H7N5
SMILES:	Nc1cc(N)nc(N)n1
Mol. weight [g/mol]:	125.13

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.10		Crippen Method
logp	-0.777		Crippen Method
mcvol	93.360	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	125.40	kJ/mol	298.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	2.47e-04	kPa	403.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines

pvap	7.14e-05	kPa	391.14	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	9.48e-05	kPa	393.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	8.89e-05	kPa	393.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	8.51e-05	kPa	393.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	1.10e-04	kPa	395.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	1.07e-04	kPa	395.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines

pvap	1.00e-04	kPa	395.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	1.41e-04	kPa	397.13	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	1.31e-04	kPa	397.13	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	1.24e-04	kPa	397.13	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	1.67e-04	kPa	399.13	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	1.66e-04	kPa	399.13	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines

pvap	1.48e-04	kPa	399.13	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	2.00e-04	kPa	401.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	1.88e-04	kPa	401.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	1.86e-04	kPa	401.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	7.31e-05	kPa	391.14	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	2.37e-04	kPa	403.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines

pvap	2.15e-04	kPa	403.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	2.92e-04	kPa	405.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	2.87e-04	kPa	405.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	2.58e-04	kPa	405.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	3.45e-04	kPa	407.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	3.16e-04	kPa	407.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines

pvap	3.19e-04	kPa	407.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	3.93e-04	kPa	409.12	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	4.07e-04	kPa	409.12	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	3.75e-04	kPa	409.12	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	4.84e-04	kPa	411.12	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	4.87e-04	kPa	411.12	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines

pvap	4.39e-04	kPa	411.12	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	5.93e-04	kPa	413.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	5.40e-04	kPa	413.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	5.36e-04	kPa	413.15	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines
pvap	7.42e-05	kPa	391.14	Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:**

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

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Aromaticity and stability going in opposite directions: An energetic, structural, magnetic and electronic study of aminopyrimidines:**

<https://www.doi.org/10.1016/j.jct.2012.05.015>

# Legend

<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pvap:</b>	Vapor pressure

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