

3-Amino-1,2,4-triazine

Other names:	1,2,4-Triazin-3-amine as-Triazine, 3-amino- 3-Amino-as-triazine 1,2,4-triazin-3-ylamine
Inchi:	InChI=1S/C3H4N4/c4-3-5-1-2-6-7-3/h1-2H,(H2,4,5,7)
InchiKey:	MJIWQHRXSLOUJN-UHFFFAOYSA-N
Formula:	C3H4N4
SMILES:	<chem>N=c1nncc[nH]1</chem>
Mol. weight [g/mol]:	96.09
CAS:	1120-99-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.21		Crippen Method
logp	-1.198		Crippen Method
mcvol	69.290	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120996&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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