

1,3,5-Triazin-2(1H)-one, 4,6-diamino-

Other names:	s-Triazin-2-ol, 4,6-diamino- Ammelin Ammeline 2,4-Diamino-1,3,5-triazin-6-one 4,6-Diamino-1,3,5-triazin-2(1H)-one 4,6-Diamino-1,3,5-triazin-2-ol Ammeline, (4,6-diamino-5-triazin-2-ol)
Inchi:	InChI=1S/C3H5N5O/c4-1-6-2(5)8-3(9)7-1/h(H5,4,5,6,7,8,9)
InchiKey:	MASBWURJQFFLOO-UHFFFAOYSA-N
Formula:	C3H5N5O
SMILES:	<chem>Nc1nc(N)[nH]c(=O)n1</chem>
Mol. weight [g/mol]:	127.10
CAS:	645-92-1

Physical Properties

Property code	Value	Unit	Source
chs	-1595.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-300.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	1.09		Crippen Method
logp	-2.153		Crippen Method
mcvol	85.140	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=C645921&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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