

As-triazine-6-carboxylic acid, 3-amino-5-hydroxy-

Inchi:	InChI=1S/C4H4N4O3/c5-4-6-2(9)1(3(10)11)7-8-4/h(H,10,11)(H3,5,6,8,9)
InchiKey:	WWRSBGQVXOZNDV-UHFFFAOYSA-N
Formula:	C4H4N4O3
SMILES:	<chem>Nc1nnc(C(=O)O)c(O)n1</chem>
Mol. weight [g/mol]:	156.10
CAS:	116496-93-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.01		Crippen Method
logp	-1.142		Crippen Method
mcvol	96.690	ml/mol	McGowan Method

Sources

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=C116496936&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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