

4-Pyridinamine, 3,5-dinitro-

Other names:	4-Amino-3,5-dinitropyridine Pyridine, 4-amino-3,5-dinitro-
Inchi:	InChI=1S/C5H4N4O4/c6-5-3(8(10)11)1-7-2-4(5)9(12)13/h1-2H,(H2,6,7)
InchiKey:	IEUQRKITTGSLJL-UHFFFAOYSA-N
Formula:	C5H4N4O4
SMILES:	<chem>Nc1c([N+](=O)[O-])cncc1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	184.11
CAS:	31793-29-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	0.480		Crippen Method
mcvol	112.350	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31793290&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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