2,6-Pyridinediamine, 3,5-dinitro-

Other names:	2,6-Diamino-3,5-dinitropyridine
	3,5-Dinitro-2,6-diaminopyridine
	3,5-Dinitro-2,6-pyridinediamine
Inchi:	InChI=1S/C5H5N5O4/c6-4-2(9(11)12)1-3(10(13)14)5(7)8-4/h1H,(H4,6,7,8)
InchiKey:	ZLJZDCVHRYAHAW-UHFFFAOYSA-N
Formula:	C5H5N5O4
SMILES:	N=c1[nH]c(N)c([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	199.12
CAS:	34981-11-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.62		Crippen Method
logp	-0.589		Crippen Method
mcvol	122.330	ml/mol	McGowan Method
tf	595.15	K	Solubility of 2,6-Diamino-3,5-dinitropyridine and 2,5-Dihydroxyterephthalic Acid in N,N-Dimethylformamide, Dimethylsulfoxide, Ethanol, and Methanol, N,N-Dimethylacetamide, and Acetic Acid

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34981118&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of 2,6-Diamino-3,5-dinitropyridine and 2,5-Dihydroxyterephthalic Acid in N,N-Dimethylformamide, Dimethylsulfoxide, Ethanol, and Methanol, N,N-Dimethylacetamide, and Acetic Acid:	https://www.doi.org/10.1021/je900367v

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point