

4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-

Other names:	Orotic acid, 5-amino- Orothric acid, 5-amino- 5-Aminoorotic acid 5-Amino-2,6-dioxo-1,2,3,6-tetrahydro-pyrimidine-4-carboxylic acid 5-Amino-2,6-dioxo-1,2,3,6-tetrahydro-4-pyrimidinecarboxylic acid 5-Amino-2,6-dihydroxy-4-pyrimidinecarboxylic acid NSC 43249 5-amino-2,6-dioxo-1,2,3,4-tetrahydropyrimidine-4-carboxylic acid
Inchi:	InChI=1S/C5H5N3O4/c6-1-2(4(10)11)7-5(12)8-3(1)9/h6H2,(H,10,11)(H2,7,8,9,12)
InchiKey:	HWCXJKLFOSBVLH-UHFFFAOYSA-N
Formula:	C5H5N3O4
SMILES:	<chem>Nc1c(C(=O)O)[nH]c(=O)[nH]c1=O</chem>
Mol. weight [g/mol]:	171.11
CAS:	7164-43-4

Physical Properties

Property code	Value	Unit	Source
log10ws	1.55		Crippen Method
logp	-2.620		Crippen Method
mvol	106.670	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=C7164434&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.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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