

Orotic acid

Other names:	1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidinecarboxylic acid 2,6-Dihydroxy-4-pyrimidinecarboxylic acid 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-50887-69-9 (hydrate) 6-Carboxyuracil 6-Uracilcarboxylic acid Animal galactose factor NSC 9791 Orodin Oropur Orotonin Orotosan Orotsaeure Oroturic Orotyl Vitamin B13 Whey factor
Inchi:	InChI=1S/C5H4N2O4/c8-3-1-2(4(9)10)6-5(11)7-3/h1H,(H,9,10)(H2,6,7,8,11)
InchiKey:	PXQPEWDEAKTCGB-UHFFFAOYSA-N
Formula:	C5H4N2O4
SMILES:	O=C(O)c1cc(=O)[nH]c(=O)[nH]1
Mol. weight [g/mol]:	156.10
CAS:	65-86-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.93		Aqueous Solubility Prediction Method
logp	-2.202		Crippen Method
mcvol	96.690	ml/mol	McGowan Method
tf	616.94	K	Aqueous Solubility Prediction Method

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C65861&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

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

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