

Pyrido[3,4-d]pyrimidine-2,4(1H,3H)-dione

Inchi:	InChI=1S/C7H5N3O2/c11-6-4-1-2-8-3-5(4)9-7(12)10-6/h1-3H,(H2,9,10,11,12)
InchiKey:	MNNWQAIAFUMNOS-UHFFFAOYSA-N
Formula:	C7H5N3O2
SMILES:	O=c1[nH]c(=O)c2ccncc2[nH]1
Mol. weight [g/mol]:	163.13
CAS:	21038-67-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.32		Crippen Method
logp	-1.352		Crippen Method
mcvol	107.950	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C21038675&Units=SI

Legend

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

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<https://www.chemeo.com/cid/25-709-7/Pyrido-3-4-d-pyrimidine-2-4-1H-3H-dione.pdf>

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