Alloxazine

Other names:	Benzo(g)pteridine-2,4(1H,3H)-dione
	Alloxazin
	1,2,3,4-tetrahydrobenzopteridine-2,4-dione
Inchi:	InChI=1S/C10H6N4O2/c15-9-7-8(13-10(16)14-9)12-6-4-2-1-3-5(6)11-7/h1-4H,(H2,12,13,
InchiKey:	HAUGRYOERYOXHX-UHFFFAOYSA-N
Formula:	C10H6N4O2
SMILES:	Oc1nc(O)c2nc3ccccc3nc2n1
Mol. weight [g/mol]:	214.18
CAS:	490-59-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	0.984		Crippen Method
mcvol	140.740	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C490595&Units=SI
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

Legend

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

Latest version available from:
https://www.chemeo.com/cid/83-507-7/Alloxazine.pdf

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