Lumazine

Other names:	2,4(1H,3H)-Pteridinedione
	2,4(3H,8H)-Pteridinedione
	2,4-Dihydroxypteridine
	2,4-Pteridinediol
	Lumazin
	Pteridinedione, 2,4(1h,3h)-
	pteridine-2,4-diol monohydrate
Inchi:	InChI=1S/C6H4N4O2/c11-5-3-4(8-2-1-7-3)9-6(12)10-5/h1-2H,(H2,8,9,10,11,12)
InchiKey:	UYEUUXMDVNYCAM-UHFFFAOYSA-N
Formula:	C6H4N4O2
SMILES:	O=c1[nH]c(=O)c2nccnc2[nH]1
Mol. weight [g/mol]:	164.12
CAS:	487-21-8

Physical Properties

Property code	Value	Unit	Source
ie	9.20	eV	NIST Webbook
log10ws	-0.09		Crippen Method
logp	-1.957		Crippen Method
mcvol	103.840	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C487218&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

ie:	Ionization energy

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