

Lumichrome

Other names:	Benzo[g]pteridine-2,4(1H,3H)-dione, 7,8-dimethyl-Alloxazine, 7,8-dimethyl-Riboflavin lumichrome 7,8-Dimethylalloxazine Lumichrome (I) 7,8-dimethylbenzo[g]pteridine-2,4(1H,3H)-dione
Inchi:	InChI=1S/C12H10N4O2/c1-5-3-7-8(4-6(5)2)14-10-9(13-7)11(17)16-12(18)15-10/h3-4H,1
InchiKey:	ZJTJUUVIJVLLGSP-UHFFFAOYSA-N
Formula:	C12H10N4O2
SMILES:	<chem>Cc1cc2nc3[nH]c(=O)[nH]c(=O)c3nc2cc1C</chem>
Mol. weight [g/mol]:	242.23
CAS:	1086-80-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	-0.187		Crippen Method
mcvol	168.920	ml/mol	McGowan Method

Sources

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=C1086802&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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