

Lumiflavine

Other names:	Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-Lumiflavin Lumilactoflavin 7,8,10-Trimethylisoalloxazine Lumiflavin (III) 7,8,10-trimethylbenzo[g]pteridine-2,4(3H,10H)-dione
Inchi:	InChI=1S/C13H12N4O2/c1-6-4-8-9(5-7(6)2)17(3)11-10(14-8)12(18)16-13(19)15-11/h4-5
InchiKey:	KPDQZGKJTRBGU-UHFFFAOYSA-N
Formula:	C13H12N4O2
SMILES:	<chem>Cc1cc2nc3c(=O)[nH]c(=O)nc-3n(C)c2cc1C</chem>
Mol. weight [g/mol]:	256.26
CAS:	1088-56-8

Physical Properties

Property code	Value	Unit	Source
ie	8.72	eV	NIST Webbook
log10ws	-5.13		Crippen Method
logp	0.257		Crippen Method
mcvol	183.010	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=C1088568&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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