Benzo[g]pteridine-2,4(3H,10H)-dione, 3,7,8,10-tetramethyl-

Other names: Isoalloxazine, 3,7,8,10-tetramethyl-
3-Methyllumiflavin
3-Methyllumiflavine
3,6,7,9-Tetramethylisoalloxazine
3,7,8,10-Tetramethylbenzo[g]pteridine-2,4(3H,10H)-dione

Inchi: InChI=1S/C14H14N4O2/c1-7-5-9-10(6-8(7)2)17(3)12-11(15-9)13(19)18(4)14(20)16-12/h5

InchiKey: DSUJCACXEBHAAS-UHFFFAOYSA-N

Formula: C14H14N4O2

SMILES: Cc1cc2nc3c(=O)n(C)c(=O)nc-3n(C)c2cc1C

Mol. weight [g/mol]: 270.29

CAS: 18636-32-3

Physical Properties

Property code	Value	Unit	Source
ie	8.22	eV	NIST Webbook
log10ws	-7.20		Crippen Method
logp	0.749		Crippen Method
mcvol	197.100	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=C18636323&Units=SI

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume