

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

Other names:	Isoalloxazine, 3,7,8,10-tetramethyl-3-Methylumiflavin 3-Methylumiflavine 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/h
InchiKey:	DSUJCACXEBHAAS-UHFFFAOYSA-N
Formula:	C14H14N4O2
SMILES:	<chem>Cc1cc2nc3c(=O)n(C)c(=O)nc-3n(C)c2cc1C</chem>
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/ci9903071
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

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