# Lumiflavine

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|---|---|
| **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:** | KPDQZGKJTJRBGU-UHFFFAOYSA-N |
| **Formula:** | C13H12N4O2 |
| **SMILES:** | Cc1cc2nc3c(=O)[nH]c(=O)nc-3n(C)c2cc1C |
| **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

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| **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/ci990307l |

# Legend

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

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume