2,4(1H,3H)-Pteridinedione, 8-methyl-

Other names: Lumazine, 8-methyl-
Inchi: InChI=1S/C7H6N4O2/c1-11-3-2-8-4-5(11)9-7(13)10-6(4)12/h2-3H,1H3,(H,10,12,13)
InchiKey: FEVFINCNKRMCDL-UHFFFAOYSA-N
Formula: C7H6N4O2
SMILES: Cn1ccnc2c(=O)[nH]c(=O)nc1-2
Mol. weight [g/mol]: 178.15
CAS: 13300-38-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	-1.514		Crippen Method
mcvol	117.930	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=C13300384&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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