

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:	<chem>Cn1ccnc2c(=O)[nH]c(=O)nc1-2</chem>
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/ci9903071

Legend

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

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