

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

Other names:	2,4(1H,3H)-Pteridinedione
	2,4(3H,8H)-Pteridinedione
	2,4-Dihydroxypteridine
	2,4-Pteridinediol
	Lumazin
	Pteridinedione, 2,4(1h,3h)- pteridine-2,4-diol monohydrate
Inchi:	InChI=1S/C6H4N4O2/c11-5-3-4(8-2-1-7-3)9-6(12)10-5/h1-2H,(H2,8,9,10,11,12)
InchiKey:	UYEUUXMDVNYCAM-UHFFFAOYSA-N
Formula:	C6H4N4O2
SMILES:	O=c1[nH]c(=O)c2nccnc2[nH]1
Mol. weight [g/mol]:	164.12

Physical Properties

Property code	Value	Unit	Source
ie	9.20	eV	NIST Webbook
logp	-1.957		Crippen Method
mcvol	103.840	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C487218&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/37-507-8/2-4-1H-3H-Pteridinedione.pdf>

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