

2-MERCAPTO-4-PTERIDINOL

Other names:	4(1H)-Pteridinone, 2,3-dihydro-2-thioxo-2-mercaptopteridin-4-ol
Inchi:	InChI=1S/C6H4N4OS/c11-5-3-4(8-2-1-7-3)9-6(12)10-5/h1-2H,(H2,8,9,10,11,12)
InchiKey:	VSPCYUNOZPCHLL-UHFFFAOYSA-N
Formula:	C6H4N4OS
SMILES:	Oc1nc(S)nc2nccnc12
Mol. weight [g/mol]:	180.19

Physical Properties

Property code	Value	Unit	Source
logp	0.414		Crippen Method
mcvol	114.320	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C52023480&Units=SI>

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/96-877-3/2-MERCAPTO-4-PTERIDINOL.pdf>

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