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