2-Amino-3,5,7,8-tetrahydro-4,6-pteridinedione

Inchi: InChI=1S/C6H7N5O2/c7-6-10-4-3(5(13)11-6)9-2(12)1-8-4/h1H2,(H,9,12)(H4,7,8,10,11,13

InchiKey: JLRDKNBQJOODBP-UHFFFAOYSA-N

Formula: C6H7N5O2

SMILES: Nc1nc2c(c(=O)[nH]1)NC(=O)CN2

Mol. weight [g/mol]: 181.15

CAS: 1011-23-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.80		Crippen Method
logp	-1.766		Crippen Method
mcvol	118.120	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=C1011230&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