

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

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