2-AMINO-4-HYDROXYPTERIDINE-6-CARBOXYLIC ACID

Other names: Pterine-6-carboxylic acid
2-Amino-4-hydroxypteridine-6-carboxylic acid
6-Pteridinecarboxylic acid, 2-amino-1,4-dihydro-4-oxo-
2-amino-1,4-dihydro-4-oxopteridine-6-carboxylic acid

Inchi: InChI=1S/C7H5N5O3/c8-7-11-4-3(5(13)12-7)10-2(1-9-4)6(14)15/h1H,(H,14,15)(H3,8,9,1

InchiKey: QABAUCFGPWONOG-UHFFFAOYSA-N

Formula: C7H5N5O3

SMILES: Nc1nc2ncc(C(=O)O)nc2c(=O)[nH]1

Mol. weight [g/mol]: 207.15

Physical Properties

Property code	Value	Unit	Source
ie	8.55	eV	Cheméo Relay (1.0)
logp	-1.488		Crippen Method
mcvol	129.480	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C948607&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

ie: Ionization energy

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume