

6-Pteridinecarboxamide, 4,7-diamino-2-phenyl-

Inchi:	InChI=1S/C13H11N7O/c14-9-7(11(16)21)17-8-10(15)18-12(20-13(8)19-9)6-4-2-1-3-5-6/h
InchiKey:	LEWFJJFRRGXGGL-UHFFFAOYSA-N
Formula:	C13H11N7O
SMILES:	<chem>N=C(O)c1nc2c(N)nc(-c3ccccc3)[nH]c-2nc1=N</chem>
Mol. weight [g/mol]:	281.27
CAS:	1230-14-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.46		Crippen Method
logp	0.435		Crippen Method
mcvol	198.480	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1230144&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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