# 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:** N=C(O)c1nc2c(N)nc(-c3ccccc3)[nH]c-2nc1=N
**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/ci990307l
**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