

Nicotinic acid, 6-[n-[(2-acetamido-3-hydro-4-oxo-6-pteridinyI)met

Inchi: InChI=1S/C17H15N7O5/c1-8(25)20-17-22-14-13(15(27)23-17)21-11(6-19-14)7-24(9(2)2
InchiKey: VXUFKCGJKUZANA-UHFFFAOYSA-N
Formula: C17H15N7O5
SMILES: CC(=O)Nc1nc2ncc(CN(C(C)=O)c3ccc(C(=O)O)cn3)nc2c(=O)[nH]1
Mol. weight [g/mol]: 397.34
CAS: 30958-64-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	-0.164		Crippen Method
mcvol	269.720	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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=C30958646&Units=SI>

Legend

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

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