

8-ethyl-5,8-dihydro-5-oxo-2-(1-piperazinyl)pyrido[1,2-a]pyrimidin-6-carboxylic acid

Other names: pipemidic acid
pyrido[2,3-d]pyrimidine-6-carboxylic acid, 8-ethyl-5,8-dihydro-5-oxo-2-(1-piperazinyl)-
Inchi: InChI=1S/C14H17N5O3/c1-2-18-8-10(13(21)22)11(20)9-7-16-14(17-12(9)18)19-5-3-15-4
InchiKey: JOHZPMXAZQZXHR-UHFFFAOYSA-N
Formula: C14H17N5O3
SMILES: CCn1cc(C(=O)[O-])c(=O)c2cnc(N3CC[NH2+]CC3)nc21
Mol. weight [g/mol]: 303.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Cheméo Relay (1.0)
logp	-2.442		Crippen Method
mcvol	217.250	ml/mol	McGowan Method
tf	538.15	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Determination and Correlation for Solubilities of Ofloxacin, Norfloxacin, Levofloxacin, and Ciprofloxacin, <https://www.doi.org/10.1021/je100116u>
Solubility of Ofloxacin, Norfloxacin, Levofloxacin, and Ciprofloxacin, <https://www.doi.org/10.1021/je7007044>
Norfloxacin and Pipemidic Acid in Octanol-Water (293.15 to 333.15) K: <http://link.springer.com/article/10.1007/BF02311772>
Pipemidic Acid from (293.15 to 323.15) K: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method:
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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