

4-Oxo-2-pyridinium-3-(2,4,6-trioxo-1,3-diazacyclohexylidene)-5,1-naphthoxide

Inchi: InChI=1S/C19H11N3O5/c23-15-10-6-2-3-7-11(10)16(24)14(22-8-4-1-5-9-22)12(15)13-17
InchiKey: YHKWODVVNQKJRA-UHFFFAOYSA-N
Formula: C19H11N3O5
SMILES: O=C1NC(=O)C(=C2C(=O)c3ccccc3C([O-])=C2[n+]2ccccc2)C(=O)N1
Mol. weight [g/mol]: 361.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.50		Crippen Method
logp	-0.481		Crippen Method
mcvol	242.820	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004431&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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