isoguanine

Inchi: InChI=1S/C5H5N5O/c6-3-2-4(8-1-7-2)10-5(11)9-3/h1H,(H4,6,7,8,9,10,11)
InchiKey: DRAVOWXCEBXPTN-UHFFFAOYSA-N
Formula: C5H5N5O
SMILES: Nc1nc(O)nc2nc[nH]c12
Mol. weight [g/mol]: 151.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Aqueous Solubility Prediction Method
log10ws	-3.40		Estimated Solubility Method
logp	-0.841		Crippen Method
mcvol	98.160	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.