

7-methoxypteridine

Inchi: InChI=1S/C7H6N4O/c1-12-6-3-9-5-2-8-4-10-7(5)11-6/h2-4H,1H3
InchiKey: NMUINCUJOZFODB-UHFFFAOYSA-N
Formula: C7H6N4O
SMILES: COc1cnc2cncnc2n1
Mol. weight [g/mol]: 162.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.14		Aqueous Solubility Prediction Method
log10ws	-0.91		Estimated Solubility Method
log10ws	-0.91		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.428		Crippen Method
mcvol	112.060	ml/mol	McGowan Method

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous and cosolvent solubility data for drug-like organic compounds: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/>
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Legend

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

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