7-Methylpteridine

Inchi: InChI=1S/C7H6N4/c1-5-2-9-6-3-8-4-10-7(6)11-5/h2-4H,1H3
InchiKey: KOCYTWBTXZOUFS-UHFFFAOYSA-N
Formula: C7H6N4
SMILES: Cc1cnc2cncnc2n1
Mol. weight [g/mol]: 146.15

Physical Properties

Property code	Value	Unit	Source
log10ws	0.06		Aqueous Solubility Prediction Method
log10ws	-0.85		Estimated Solubility Method
log10ws	-0.85		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.728		Crippen Method
mcvol	106.190	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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
Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

Legend

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