7-Chloropteridine

Inchi: InChI=1S/C6H3ClN4/c7-5-2-9-4-1-8-3-10-6(4)11-5/h1-3H
InchiKey: AANUQVPVSJJCRI-UHFFFAOYSA-N
Formula: C6H3ClN4
SMILES: Clc1cnc2cncnc2n1
Mol. weight [g/mol]: 166.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.87		Aqueous Solubility Prediction Method
log10ws	-0.88		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	1.073		Crippen Method
mcvol	104.340	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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/ci990307l

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.