

6-Chloropteridine

Inchi: InChI=1S/C6H3ClN4/c7-5-2-9-6-4(11-5)1-8-3-10-6/h1-3H
InchiKey: YAVYBQFUSWPIQK-UHFFFAOYSA-N
Formula: C6H3ClN4
SMILES: Clc1cnc2ncncc2n1
Mol. weight [g/mol]: 166.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.87		Aqueous Solubility Prediction Method
log10ws	-1.12		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/AqueousDataset002.xlsx>

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>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/104-071-7/6-Chloropteridine.pdf>

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