

2-chloropteridine

Inchi:	InChI=1S/C6H3ClN4/c7-6-10-3-4-5(11-6)9-2-1-8-4/h1-3H
InchiKey:	JISQBJRFTCXDEO-UHFFFAOYSA-N
Formula:	C6H3ClN4
SMILES:	Clc1ncc2nccnc2n1
Mol. weight [g/mol]:	166.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.70		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	1.073		Crippen Method
mcvol	104.340	ml/mol	McGowan Method

Sources

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

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