6-methoxypteridine

Inchi: InChI=1S/C7H6N4O/c1-12-6-3-9-7-5(11-6)2-8-4-10-7/h2-4H,1H3
InchiKey: AWIJPALBOQNRBS-UHFFFAOYSA-N
Formula: C7H6N4O
SMILES: COc1cnc2ncncc2n1
Mol. weight [g/mol]: 162.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.14		Estimated Solubility Method
logp	0.428		Crippen Method
mcvol	112.060	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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