O-(4-methylphenyl) diamidothiophosphate

Inchi: InChI=1S/C7H11N2OPS/c1-6-2-4-7(5-3-6)10-11(8,9)12/h2-5H,1H3,(H4,8,9,12)
InchiKey: LEFQEXODSQORQA-UHFFFAOYSA-N
Formula: C7H11N2OPS
SMILES: Cc1ccc(OP(N)(N)=S)cc1
Mol. weight [g/mol]: 202.21

Physical Properties

Property code	Value	Unit	Source
log10ws	1.23		Crippen Method
logp	1.516		Crippen Method
mcvol	148.370	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001208&Units=SI

Legend

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