O-(2-cyclohexylphenyl) o-methyl amidothiophosphate

Inchi: InChI=1S/C13H20NO2PS/c1-15-17(14,18)16-13-10-6-5-9-12(13)11-7-3-2-4-8-11/h5-6,9-

InchiKey: BJPSPQKRHJVJEC-UHFFFAOYSA-N

Formula: C13H20NO2PS

SMILES: COP(N)(=S)Oc1ccccc1C1CCCCC1

Mol. weight [g/mol]: 285.34

CAS: 109105-43-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.70		Crippen Method
logp	3.943		Crippen Method
mcvol	217.940	ml/mol	McGowan Method

Sources

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=C109105433&Units=SI

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