

O-(2-cyclohexylphenyl) o-methylamidothiophosphate

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

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<https://www.chemeo.com/cid/80-091-2/O-2-cyclohexylphenyl-o-methyl-amidothiophosphate.pdf>

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