5-Methoxy-2(1-phenyl-5-mercaptotetrazole)-quino

Inchi: InChI=1S/C14H10N4O3S/c1-21-12-7-11(20)13(8-10(12)19)22-14-15-16-17-18(14)9-5-3-
InchiKey: CGRQOOHXEFZOLT-UHFFFAOYSA-N
Formula: C14H10N4O3S
SMILES: COC1=CC(=O)C(Sc2nnnn2-c2ccccc2)=CC1=O
Mol. weight [g/mol]: 314.32
CAS: 95980-60-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	1.320		Crippen Method
mcvol	210.720	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=C95980602&Units=SI

Legend

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