1,2,4-Triazol-5(4H)-thione, 4-allyl-3-phenyl-

Inchi: InChI=1S/C11H11N3S/c1-2-8-14-10(12-13-11(14)15)9-6-4-3-5-7-9/h2-7H,1,8H2,(H,13,15
InchiKey: ZLSZMYUZPQLFCY-UHFFFAOYSA-N
Formula: C11H11N3S
SMILES: C=CCn1c(-c2ccccc2)n[nH]c1=S
Mol. weight [g/mol]: 217.29
CAS: 23714-53-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.44		Crippen Method
logp	2.312		Crippen Method
mcvol	164.620	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=C23714536&Units=SI

Legend

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