

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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/34-422-5/1-2-4-Triazol-5-4H-thione-4-allyl-3-phenyl.pdf>

Generated by Cheméo on 2024-05-16 18:28:14.763991952 +0000 UTC m=+18173343.684569263.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.