

3-Methyl-4-phenyl-4-thiazoline-2-thione

Inchi:	InChI=1S/C10H9NS2/c1-11-9(7-13-10(11)12)8-5-3-2-4-6-8/h2-7H,1H3
InchiKey:	YGZDFPNBMUHUON-UHFFFAOYSA-N
Formula:	C10H9NS2
SMILES:	Cn1c(-c2ccccc2)csc1=S
Mol. weight [g/mol]:	207.31
CAS:	21402-19-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.97		Crippen Method
logp	3.483		Crippen Method
mcvol	151.220	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=C21402197&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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