

1-(4-Methoxyphenyl)imidazoline-2-thione

Inchi:	InChI=1S/C10H10N2OS/c1-13-9-4-2-8(3-5-9)12-7-6-11-10(12)14/h2-7H,1H3,(H,11,14)
InchiKey:	LIEBCNQPMNARMP-UHFFFAOYSA-N
Formula:	C10H10N2OS
SMILES:	COc1ccc(-n2cc[nH]c2=S)cc1
Mol. weight [g/mol]:	206.26
CAS:	17452-14-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	2.062		Crippen Method
mcvol	150.720	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17452141&Units=SI
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

Legend

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

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