

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

Inchi:	InChI=1S/C9H7BrN2S/c10-7-1-3-8(4-2-7)12-6-5-11-9(12)13/h1-6H,(H,11,13)
InchiKey:	ZKPXIPSWVWPFDF-UHFFFAOYSA-N
Formula:	C9H7BrN2S
SMILES:	S=c1[nH]ccn1-c1ccc(Br)cc1
Mol. weight [g/mol]:	255.13
CAS:	17452-23-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.36		Crippen Method
logp	2.815		Crippen Method
mcvol	148.260	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17452232&Units=SI
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

Legend

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

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