

1-(3-Fluorophenyl)imidazoline-2-thione

Inchi:	InChI=1S/C9H7FN2S/c10-7-2-1-3-8(6-7)12-5-4-11-9(12)13/h1-6H,(H,11,13)
InchiKey:	BMCFDCBHCVAIC-UHFFFAOYSA-N
Formula:	C9H7FN2S
SMILES:	Fc1cccc(-n2cc[nH]c2=S)c1
Mol. weight [g/mol]:	194.23
CAS:	17452-26-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	2.192		Crippen Method
mcvol	132.530	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17452265&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/31-751-3/1-3-Fluorophenyl-imidazoline-2-thione.pdf>

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