

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

Inchi:	InChI=1S/C10H7F3N2S/c11-10(12,13)7-2-1-3-8(6-7)15-5-4-14-9(15)16/h1-6H,(H,14,16)
InchiKey:	FQMZFHKIYYCCAX-UHFFFAOYSA-N
Formula:	C10H7F3N2S
SMILES:	FC(F)(F)c1cccc(-n2cc[nH]c2=S)c1
Mol. weight [g/mol]:	244.24
CAS:	17452-08-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Crippen Method
logp	3.072		Crippen Method
mcvol	150.160	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=C17452083&Units=SI

Legend

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

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