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

Inchi: InChI=1S/C10H7F3N2S/c11-10(12,13)7-3-1-2-4-8(7)15-6-5-14-9(15)16/h1-6H,(H,14,16)
InchiKey: SHEVDRLIPIJLJW-UHFFFAOYSA-N
Formula: C10H7F3N2S
SMILES: FC(F)(F)c1ccccc1-n1cc[nH]c1=S
Mol. weight [g/mol]: 244.24
CAS: 25372-17-2

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25372172&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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