

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

<b>Inchi:</b>	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)
<b>InchiKey:</b>	SHEVDRLIPIJLJW-UHFFFAOYSA-N
<b>Formula:</b>	C10H7F3N2S
<b>SMILES:</b>	FC(F)(F)c1ccccc1-n1cc[nH]c1=S
<b>Mol. weight [g/mol]:</b>	244.24
<b>CAS:</b>	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

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C25372172&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25372172&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/117-910-1/1-2-Trifluoromethylphenyl-imidazoline-2-thione.pdf>

Generated by Cheméo on 2024-05-02 17:05:17.270019206 +0000 UTC m=+16958766.190596521.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.