

# 2-(2-Chloro-1,1,2-trifluoroethylthio)phenyl isothiocyanate

**Inchi:** InChI=1S/C9H5ClF3NS2/c10-8(11)9(12,13)16-7-4-2-1-3-6(7)14-5-15/h1-4,8H  
**InchiKey:** GDPSMRKGJDVUMB-UHFFFAOYSA-N  
**Formula:** C9H5ClF3NS2  
**SMILES:** FC(Cl)C(F)(F)Sc1ccccc1N=C=S  
**Mol. weight [g/mol]:** 283.72  
**CAS:** 207919-07-1

## Physical Properties

Property code	Value	Unit	Source
hf	-296.19	kJ/mol	Joback Method
hvap	56.07	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.640		Crippen Method
mcvol	165.540	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
tb	683.28	K	Joback Method
tc	941.91	K	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C207919071&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** Log10 of Water solubility in mol/l

<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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