

# 2,4,6-Trifluorophenyl isothiocyanate

<b>Inchi:</b>	InChI=1S/C7H2F3NS/c8-4-1-5(9)7(11-3-12)6(10)2-4/h1-2H
<b>InchiKey:</b>	JPISVBDECFJHDB-UHFFFAOYSA-N
<b>Formula:</b>	C7H2F3NS
<b>SMILES:</b>	Fc1cc(F)c(N=C=S)c(F)c1
<b>Mol. weight [g/mol]:</b>	189.16
<b>CAS:</b>	206761-91-3

## Physical Properties

Property code	Value	Unit	Source
hf	-289.95	kJ/mol	Joback Method
hvap	43.43	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.838		Crippen Method
mcvol	108.770	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	544.94	K	Joback Method
tc	773.87	K	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C206761913&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C206761913&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	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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