

# p-Trifluoromethylphenylisothiocyanate

<b>Inchi:</b>	InChI=1S/C8H4F3NS/c9-8(10,11)6-1-3-7(4-2-6)13-5-12/h1-4H
<b>InchiKey:</b>	WRBJDWSTNUOWMF-UHFFFAOYSA-N
<b>Formula:</b>	C8H4F3NS
<b>SMILES:</b>	N#CSc1ccc(C(F)(F)F)cc1
<b>Mol. weight [g/mol]:</b>	203.18
<b>CAS:</b>	1645-65-4

## Physical Properties

Property code	Value	Unit	Source
gf	-296.03	kJ/mol	Joback Method
hf	-373.72	kJ/mol	Joback Method
hfus	17.59	kJ/mol	Joback Method
hvap	49.89	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.279		Crippen Method
mcvol	122.860	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
tb	579.54	K	Joback Method
tc	810.93	K	Joback Method
tf	322.44	K	Joback Method
vc	0.498	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.92	J/molxK	579.54	Joback Method
cpg	281.05	J/molxK	618.10	Joback Method
cpg	289.38	J/molxK	656.67	Joback Method
cpg	296.96	J/molxK	695.23	Joback Method
cpg	303.85	J/molxK	733.80	Joback Method
cpg	310.09	J/molxK	772.36	Joback Method
cpg	315.72	J/molxK	810.93	Joback Method

# Sources

<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>
<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1645654&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1645654&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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