

# 4-Fluorophenyl trifluoromethyl sulphide

<b>Inchi:</b>	InChI=1S/C7H4F4S/c8-5-1-3-6(4-2-5)12-7(9,10)11/h1-4H
<b>InchiKey:</b>	BTKQCAUEXFTVNT-UHFFFAOYSA-N
<b>Formula:</b>	C7H4F4S
<b>SMILES:</b>	Fc1ccc(SC(F)(F)F)cc1
<b>Mol. weight [g/mol]:</b>	196.16
<b>CAS:</b>	940-76-1

## Physical Properties

Property code	Value	Unit	Source
gf	-632.44	kJ/mol	Joback Method
hf	-714.07	kJ/mol	Joback Method
hfus	16.57	kJ/mol	Joback Method
hvap	36.37	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.438		Crippen Method
mcvol	109.160	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
tb	453.85	K	Joback Method
tc	659.12	K	Joback Method
tf	246.77	K	Joback Method
vc	0.434	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.36	J/molxK	453.85	Joback Method
cpg	229.71	J/molxK	488.06	Joback Method
cpg	239.31	J/molxK	522.27	Joback Method
cpg	248.22	J/molxK	556.48	Joback Method
cpg	256.46	J/molxK	590.70	Joback Method
cpg	264.06	J/molxK	624.91	Joback Method
cpg	271.06	J/molxK	659.12	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C940761&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C940761&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>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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