

# 3,5-Bis(trifluoromethyl)thiophenol

<b>Inchi:</b>	InChI=1S/C8H4F6S/c9-7(10,11)4-1-5(8(12,13)14)3-6(15)2-4/h1-3,15H
<b>InchiKey:</b>	KCAQWPZIMLEAF-UHFFFAOYSA-N
<b>Formula:</b>	C8H4F6S
<b>SMILES:</b>	FC(F)(F)c1cc(S)cc(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	246.17
<b>CAS:</b>	130783-02-7

## Physical Properties

Property code	Value	Unit	Source
gf	-1024.16	kJ/mol	Joback Method
hf	-1150.54	kJ/mol	Joback Method
hfus	17.43	kJ/mol	Joback Method
hvap	36.25	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.013		Crippen Method
mcvol	126.790	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
tb	471.10	K	Joback Method
tc	666.67	K	Joback Method
tf	276.22	K	Joback Method
vc	0.515	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.98	J/molxK	471.10	Joback Method
cpg	288.90	J/molxK	503.69	Joback Method
cpg	298.96	J/molxK	536.29	Joback Method
cpg	308.21	J/molxK	568.88	Joback Method
cpg	316.70	J/molxK	601.48	Joback Method
cpg	324.48	J/molxK	634.07	Joback Method
cpg	331.59	J/molxK	666.67	Joback Method

# Sources

<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=C130783027&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C130783027&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>

# 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>mcvol:</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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