

# Trifluoromethanesulfonyl chloride

<b>Other names:</b>	Methanesulfonyl chloride, trifluoro-trifluoromethanesulphonyl chloride
<b>Inchi:</b>	InChI=1S/CCIF3O2S/c2-8(6,7)1(3,4)5
<b>InchiKey:</b>	GRGCWBWNLSTIEN-UHFFFAOYSA-N
<b>Formula:</b>	CCIF3O2S
<b>SMILES:</b>	O=S(=O)(Cl)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	168.52
<b>CAS:</b>	421-83-0

## Physical Properties

Property code	Value	Unit	Source
gf	-1104.52	kJ/mol	Joback Method
hf	-1130.14	kJ/mol	Joback Method
hfus	15.75	kJ/mol	Joback Method
hvap	37.09	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.075		Crippen Method
mvol	70.590	ml/mol	McGowan Method
pc	5809.41	kPa	Joback Method
tb	305.50 ± 0.50	K	NIST Webbook
tc	455.24	K	Joback Method
tf	173.70	K	Joback Method
vc	0.309	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.79	J/mol×K	302.07	Joback Method
cpg	119.40	J/mol×K	327.60	Joback Method
cpg	123.80	J/mol×K	353.13	Joback Method
cpg	127.97	J/mol×K	378.66	Joback Method
cpg	131.93	J/mol×K	404.19	Joback Method
cpg	135.67	J/mol×K	429.72	Joback Method
cpg	139.21	J/mol×K	455.24	Joback Method

# Sources

<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=C421830&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C421830&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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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