

# 2,3,6-Trifluoroaniline

<b>Inchi:</b>	InChI=1S/C6H4F3N/c7-3-1-2-4(8)6(10)5(3)9/h1-2H,10H2
<b>InchiKey:</b>	RGUGZPYMOAJLO-UHFFFAOYSA-N
<b>Formula:</b>	C6H4F3N
<b>SMILES:</b>	Nc1c(F)ccc(F)c1F
<b>Mol. weight [g/mol]:</b>	147.10
<b>CAS:</b>	67815-56-9

## Physical Properties

Property code	Value	Unit	Source
gf	-434.82	kJ/mol	Joback Method
hf	-519.59	kJ/mol	Joback Method
hfus	18.61	kJ/mol	Joback Method
hvap	41.40	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.686		Crippen Method
mcvol	86.930	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	448.64	K	Joback Method
tc	647.02	K	Joback Method
tf	306.39	K	Joback Method
vc	0.346	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.95	J/molxK	448.64	Joback Method
cpg	182.53	J/molxK	481.70	Joback Method
cpg	189.75	J/molxK	514.77	Joback Method
cpg	196.60	J/molxK	547.83	Joback Method
cpg	203.09	J/molxK	580.89	Joback Method
cpg	209.25	J/molxK	613.96	Joback Method
cpg	215.06	J/molxK	647.02	Joback Method

# Sources

<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=C67815569&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C67815569&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>

# 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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