

# 2,3,6-Trifluorobenzaldehyde

<b>Inchi:</b>	InChI=1S/C7H3F3O/c8-5-1-2-6(9)7(10)4(5)3-11/h1-3H
<b>InchiKey:</b>	XSBAHBVACIKRTG-UHFFFAOYSA-N
<b>Formula:</b>	C7H3F3O
<b>SMILES:</b>	O=Cc1c(F)ccc(F)c1F
<b>Mol. weight [g/mol]:</b>	160.09
<b>CAS:</b>	104451-70-9

## Physical Properties

Property code	Value	Unit	Source
gf	-592.37	kJ/mol	Joback Method
hf	-659.60	kJ/mol	Joback Method
hfus	18.29	kJ/mol	Joback Method
hvap	39.71	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	1.916		Crippen Method
mcvol	92.610	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
tb	447.65	K	Joback Method
tc	636.98	K	Joback Method
tf	276.40	K	Joback Method
vc	0.391	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.21	J/mol×K	447.65	Joback Method
cpg	188.57	J/mol×K	479.21	Joback Method
cpg	195.57	J/mol×K	510.76	Joback Method
cpg	202.23	J/mol×K	542.32	Joback Method
cpg	208.56	J/mol×K	573.87	Joback Method
cpg	214.56	J/mol×K	605.43	Joback Method
cpg	220.24	J/mol×K	636.98	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=C104451709&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C104451709&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>

# 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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