

# 2-Fluoro-3-(trifluoromethyl)benzaldehyde

<b>Inchi:</b>	InChI=1S/C8H4F4O/c9-7-5(4-13)2-1-3-6(7)8(10,11)12/h1-4H
<b>InchiKey:</b>	XDMZVNQKVMTCSP-UHFFFAOYSA-N
<b>Formula:</b>	C8H4F4O
<b>SMILES:</b>	O=Cc1cccc(C(F)(F)F)c1F
<b>Mol. weight [g/mol]:</b>	192.11
<b>CAS:</b>	112641-20-0

## Physical Properties

Property code	Value	Unit	Source
gf	-766.29	kJ/mol	Joback Method
hf	-873.63	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	39.16	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.657		Crippen Method
mcvol	108.470	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	461.59	K	Joback Method
tc	649.64	K	Joback Method
tf	278.16	K	Joback Method
vc	0.454	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.01	J/molxK	461.59	Joback Method
cpg	240.50	J/molxK	492.93	Joback Method
cpg	249.38	J/molxK	524.27	Joback Method
cpg	257.66	J/molxK	555.62	Joback Method
cpg	265.38	J/molxK	586.96	Joback Method
cpg	272.57	J/molxK	618.30	Joback Method
cpg	279.26	J/molxK	649.64	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=C112641200&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C112641200&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>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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