

# 2-Fluoro-5-(trifluoromethyl)phenol

<b>Inchi:</b>	InChI=1S/C7H4F4O/c8-5-2-1-4(3-6(5)12)7(9,10)11/h1-3,12H
<b>InchiKey:</b>	MCOSBFKOUQAIJS-UHFFFAOYSA-N
<b>Formula:</b>	C7H4F4O
<b>SMILES:</b>	Oc1cc(C(F)(F)F)ccc1F
<b>Mol. weight [g/mol]:</b>	180.10
<b>CAS:</b>	141483-15-0

## Physical Properties

Property code	Value	Unit	Source
gf	-820.18	kJ/mol	Joback Method
hf	-933.25	kJ/mol	Joback Method
hfus	18.23	kJ/mol	Joback Method
hvap	42.56	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.550		Crippen Method
mcvol	98.680	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	465.69	K	Joback Method
tc	664.06	K	Joback Method
tf	324.09	K	Joback Method
vc	0.346	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.03	J/molxK	465.69	Joback Method
cpg	230.34	J/molxK	498.75	Joback Method
cpg	238.84	J/molxK	531.81	Joback Method
cpg	246.62	J/molxK	564.88	Joback Method
cpg	253.72	J/molxK	597.94	Joback Method
cpg	260.22	J/molxK	631.00	Joback Method
cpg	266.17	J/molxK	664.06	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=C141483150&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C141483150&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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