

# 3-Fluoro-5-(trifluoromethyl)benzyl alcohol

<b>Inchi:</b>	InChI=1S/C8H6F4O/c9-7-2-5(4-13)1-6(3-7)8(10,11)12/h1-3,13H,4H2
<b>InchiKey:</b>	LTWAIZVPDMHGOE-UHFFFAOYSA-N
<b>Formula:</b>	C8H6F4O
<b>SMILES:</b>	OCc1cc(F)cc(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	194.13
<b>CAS:</b>	184970-29-4

## Physical Properties

Property code	Value	Unit	Source
gf	-803.59	kJ/mol	Joback Method
hf	-940.28	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	49.12	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.337		Crippen Method
mcvol	112.770	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
tb	505.11	K	Joback Method
tc	679.44	K	Joback Method
tf	296.98	K	Joback Method
vc	0.456	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.96	J/molxK	505.11	Joback Method
cpg	268.87	J/molxK	534.17	Joback Method
cpg	277.25	J/molxK	563.22	Joback Method
cpg	285.13	J/molxK	592.28	Joback Method
cpg	292.52	J/molxK	621.33	Joback Method
cpg	299.45	J/molxK	650.39	Joback Method
cpg	305.96	J/molxK	679.44	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<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=C184970294&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C184970294&amp;Units=SI</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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