

# 3-Fluorobenzoic acid, methyl ester

<b>Other names:</b>	3-F-C6H4-COOCH3 Benzoic acid, 3-fluoro-, methyl ester
<b>Inchi:</b>	InChI=1S/C8H7FO2/c1-11-8(10)6-3-2-4-7(9)5-6/h2-5H,1H3
<b>InchiKey:</b>	YXZNVLYXBIIIIOB-UHFFFAOYSA-N
<b>Formula:</b>	C8H7FO2
<b>SMILES:</b>	COC(=O)c1cccc(F)c1
<b>Mol. weight [g/mol]:</b>	154.14
<b>CAS:</b>	455-68-5

## Physical Properties

Property code	Value	Unit	Source
gf	-309.47	kJ/mol	Joback Method
hf	-424.30	kJ/mol	Joback Method
hfus	15.99	kJ/mol	Joback Method
hvap	44.68	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.612		Crippen Method
mvol	109.030	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
tb	489.66	K	Joback Method
tc	699.06	K	Joback Method
tf	291.61	K	Joback Method
vc	0.417	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.54	J/molxK	489.66	Joback Method
cpg	233.02	J/molxK	524.56	Joback Method
cpg	242.97	J/molxK	559.46	Joback Method
cpg	252.38	J/molxK	594.36	Joback Method
cpg	261.27	J/molxK	629.26	Joback Method
cpg	269.64	J/molxK	664.16	Joback Method
cpg	277.50	J/molxK	699.06	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=C455685&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C455685&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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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