

# 3-Fluorobenzoic acid, but-3-yn-2-yl ester

<b>Inchi:</b>	InChI=1S/C11H9FO2/c1-3-8(2)14-11(13)9-5-4-6-10(12)7-9/h1,4-8H,2H3
<b>InchiKey:</b>	GEWCXAXFDVCNKH-UHFFFAOYSA-N
<b>Formula:</b>	C11H9FO2
<b>SMILES:</b>	C#CC(C)OC(=O)c1cccc(F)c1
<b>Mol. weight [g/mol]:</b>	192.19

## Physical Properties

Property code	Value	Unit	Source
gf	-63.58	kJ/mol	Joback Method
hf	-199.60	kJ/mol	Joback Method
hfus	23.22	kJ/mol	Joback Method
hvap	50.83	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.004		Crippen Method
mcvol	142.700	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpola	1286.80		NIST Webbook
rinpola	1286.80		NIST Webbook
tb	547.98	K	Joback Method
tc	767.04	K	Joback Method
tf	357.39	K	Joback Method
vc	0.541	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.15	J/mol×K	547.98	Joback Method
cpg	329.53	J/mol×K	584.49	Joback Method
cpg	341.15	J/mol×K	621.00	Joback Method
cpg	352.04	J/mol×K	657.51	Joback Method
cpg	362.22	J/mol×K	694.02	Joback Method
cpg	371.71	J/mol×K	730.53	Joback Method
cpg	380.53	J/mol×K	767.04	Joback Method

# Sources

<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=U292600&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292600&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>

# 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>hvp:</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>rinp:</b>	Non-polar retention indices
<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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