

# 4-Fluorobenzoic acid, 2-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C14H11FO2/c1-10-4-2-3-5-13(10)17-14(16)11-6-8-12(15)9-7-11/h2-9H,1H3
<b>InchiKey:</b>	QAAHWSVCFIKRRO-UHFFFAOYSA-N
<b>Formula:</b>	C14H11FO2
<b>SMILES:</b>	<chem>Cc1ccccc1OC(=O)c1ccc(F)cc1</chem>
<b>Mol. weight [g/mol]:</b>	230.23

## Physical Properties

Property code	Value	Unit	Source
gf	-156.17	kJ/mol	Joback Method
hf	-323.08	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	60.97	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.353		Crippen Method
mvol	169.810	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1660.00		NIST Webbook
tb	658.60	K	Joback Method
tc	891.72	K	Joback Method
tf	398.17	K	Joback Method
vc	0.645	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.07	J/mol×K	658.60	Joback Method
cpg	436.20	J/mol×K	697.45	Joback Method
cpg	449.28	J/mol×K	736.31	Joback Method
cpg	461.35	J/mol×K	775.16	Joback Method
cpg	472.44	J/mol×K	814.01	Joback Method
cpg	482.59	J/mol×K	852.87	Joback Method
cpg	491.82	J/mol×K	891.72	Joback Method

# Sources

<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>
<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=U299053&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299053&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>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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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