

# 3-Fluorobenzoic acid, phenyl ester

<b>Inchi:</b>	InChI=1S/C13H9FO2/c14-11-6-4-5-10(9-11)13(15)16-12-7-2-1-3-8-12/h1-9H
<b>InchiKey:</b>	DIDWZIWYRUFMSZ-UHFFFAOYSA-N
<b>Formula:</b>	C13H9FO2
<b>SMILES:</b>	O=C(Oc1ccccc1)c1cccc(F)c1
<b>Mol. weight [g/mol]:</b>	216.21

## Physical Properties

Property code	Value	Unit	Source
gf	-154.96	kJ/mol	Joback Method
hf	-290.97	kJ/mol	Joback Method
hfus	22.99	kJ/mol	Joback Method
hvap	58.09	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.045		Crippen Method
mcvol	155.720	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpola	1597.00		NIST Webbook
tb	630.74	K	Joback Method
tc	867.75	K	Joback Method
tf	374.38	K	Joback Method
vc	0.590	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.72	J/mol×K	630.74	Joback Method
cpg	387.46	J/mol×K	670.24	Joback Method
cpg	400.13	J/mol×K	709.74	Joback Method
cpg	411.78	J/mol×K	749.25	Joback Method
cpg	422.45	J/mol×K	788.75	Joback Method
cpg	432.17	J/mol×K	828.25	Joback Method
cpg	441.00	J/mol×K	867.75	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=U299055&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299055&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.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>rinpol:</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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