

# 2-Fluorobenzoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

**Inchi:** InChI=1S/C12H7F9O2/c13-7-4-2-1-3-6(7)8(22)23-5-10(16,17)12(20,21)11(18,19)9(14)15  
**InchiKey:** VDYJVYYWQQNSTC-UHFFFAOYSA-N  
**Formula:** C12H7F9O2  
**SMILES:** O=C(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1ccccc1F  
**Mol. weight [g/mol]:** 354.17

## Physical Properties

Property code	Value	Unit	Source
gf	-1828.19	kJ/mol	Joback Method
hf	-2107.27	kJ/mol	Joback Method
hfus	25.23	kJ/mol	Joback Method
hvap	42.77	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.154		Crippen Method
mvol	179.550	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1332.00		NIST Webbook
rinpol	1332.00		NIST Webbook
tb	565.21	K	Joback Method
tc	731.87	K	Joback Method
tf	333.67	K	Joback Method
vc	0.747	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.75	J/mol×K	565.21	Joback Method
cpg	489.74	J/mol×K	592.99	Joback Method
cpg	500.89	J/mol×K	620.76	Joback Method
cpg	511.26	J/mol×K	648.54	Joback Method
cpg	520.90	J/mol×K	676.31	Joback Method
cpg	529.83	J/mol×K	704.09	Joback Method
cpg	538.11	J/mol×K	731.87	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.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>
<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=U354698&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354698&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>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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