

# 3-Fluorobenzoic acid, 3-methylbutyl ester

<b>Inchi:</b>	InChI=1S/C12H15FO2/c1-9(2)6-7-15-12(14)10-4-3-5-11(13)8-10/h3-5,8-9H,6-7H2,1-2H3
<b>InchiKey:</b>	CAVZEARYKBBVBP-UHFFFAOYSA-N
<b>Formula:</b>	C12H15FO2
<b>SMILES:</b>	CC(C)CCOC(=O)c1cccc(F)c1
<b>Mol. weight [g/mol]:</b>	210.24

## Physical Properties

Property code	Value	Unit	Source
gf	-278.23	kJ/mol	Joback Method
hf	-512.14	kJ/mol	Joback Method
hfus	22.83	kJ/mol	Joback Method
hvap	53.20	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.029		Crippen Method
mvol	165.390	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1457.00		NIST Webbook
rinpol	1457.00		NIST Webbook
tb	580.74	K	Joback Method
tc	782.26	K	Joback Method
tf	321.69	K	Joback Method
vc	0.635	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.33	J/molxK	580.74	Joback Method
cpg	416.88	J/molxK	614.33	Joback Method
cpg	430.65	J/molxK	647.91	Joback Method
cpg	443.66	J/molxK	681.50	Joback Method
cpg	455.91	J/molxK	715.09	Joback Method
cpg	467.43	J/molxK	748.67	Joback Method
cpg	478.23	J/molxK	782.26	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.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=U355661&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355661&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>hvpap:</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>rinppl:</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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