

# Acetic acid, (3-fluorophenyl)methyl ester

<b>Inchi:</b>	InChI=1S/C9H9FO2/c1-7(11)12-6-8-3-2-4-9(10)5-8/h2-5H,6H2,1H3
<b>InchiKey:</b>	UUPBRSSRAJMNRL-UHFFFAOYSA-N
<b>Formula:</b>	C9H9FO2
<b>SMILES:</b>	CC(=O)OCc1cccc(F)c1
<b>Mol. weight [g/mol]:</b>	168.16

## Physical Properties

Property code	Value	Unit	Source
gf	-301.05	kJ/mol	Joback Method
hf	-444.94	kJ/mol	Joback Method
hfus	18.59	kJ/mol	Joback Method
hvap	46.91	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.889		Crippen Method
mcvol	123.120	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
rinpol	1178.00		NIST Webbook
rinpol	1178.00		NIST Webbook
tb	512.54	K	Joback Method
tc	718.86	K	Joback Method
tf	302.88	K	Joback Method
vc	0.473	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.57	J/mol×K	512.54	Joback Method
cpg	276.18	J/mol×K	546.93	Joback Method
cpg	287.19	J/mol×K	581.31	Joback Method
cpg	297.62	J/mol×K	615.70	Joback Method
cpg	307.46	J/mol×K	650.08	Joback Method
cpg	316.72	J/mol×K	684.47	Joback Method
cpg	325.43	J/mol×K	718.86	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=U368722&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368722&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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