

# Acetic acid, (2,3,6-trifluorophenyl)methyl ester

<b>Inchi:</b>	InChI=1S/C9H7F3O2/c1-5(13)14-4-6-7(10)2-3-8(11)9(6)12/h2-3H,4H2,1H3
<b>InchiKey:</b>	UFIWXJARBOUIJO-UHFFFAOYSA-N
<b>Formula:</b>	C9H7F3O2
<b>SMILES:</b>	CC(=O)OCc1c(F)ccc(F)c1F
<b>Mol. weight [g/mol]:</b>	204.15

## Physical Properties

Property code	Value	Unit	Source
gf	-709.93	kJ/mol	Joback Method
hf	-860.10	kJ/mol	Joback Method
hfus	23.97	kJ/mol	Joback Method
hvap	46.59	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.167		Crippen Method
mcvol	126.660	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	1177.00		NIST Webbook
tb	521.04	K	Joback Method
tc	709.89	K	Joback Method
tf	329.10	K	Joback Method
vc	0.509	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.60	J/molxK	521.04	Joback Method
cpg	290.49	J/molxK	552.51	Joback Method
cpg	299.95	J/molxK	583.99	Joback Method
cpg	308.98	J/molxK	615.46	Joback Method
cpg	317.58	J/molxK	646.94	Joback Method
cpg	325.75	J/molxK	678.41	Joback Method
cpg	333.50	J/molxK	709.89	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=U367957&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U367957&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>
<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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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