

# Acetic acid, trifluoro-, 1,1-dimethylethyl ester

<b>Other names:</b>	Acetic acid, trifluoro-, tert-butyl ester tert-Butyl trifluoroacetate
<b>Inchi:</b>	InChI=1S/C6H9F3O2/c1-5(2,3)11-4(10)6(7,8)9/h1-3H3
<b>InchiKey:</b>	UQJLSMYQBOJUGG-UHFFFAOYSA-N
<b>Formula:</b>	C6H9F3O2
<b>SMILES:</b>	CC(C)(C)OC(=O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	170.13
<b>CAS:</b>	400-52-2

## Physical Properties

Property code	Value	Unit	Source
gf	-813.03	kJ/mol	Joback Method
hf	-1098.30 ± 6.30	kJ/mol	NIST Webbook
hfl	-1135.00 ± 4.80	kJ/mol	NIST Webbook
hfus	8.49	kJ/mol	Joback Method
hvap	36.70 ± 4.20	kJ/mol	NIST Webbook
log10ws	-1.97		Crippen Method
logp	1.890		Crippen Method
mcpvol	108.150	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
tb	356.20	K	NIST Webbook
tc	575.88	K	Joback Method
tf	236.15	K	Joback Method
vc	0.427	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.71	J/molxK	404.32	Joback Method
cpg	239.53	J/molxK	432.91	Joback Method
cpg	249.76	J/molxK	461.51	Joback Method
cpg	259.43	J/molxK	490.10	Joback Method
cpg	268.54	J/molxK	518.69	Joback Method
cpg	277.13	J/molxK	547.29	Joback Method

## Sources

<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=C400522&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C400522&amp;Units=SI</a>
<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>

## 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>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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