

# Acetic acid, trifluoro-, 2,2,2-trifluoro-1-(trifluoromethyl)ethyl ester

Other names:	Hexafluoroisopropyl trifluoroacetate Trifluoroacetic acid, 2,2,2-1-(trifluoromethyl)ethyl ester
Inchi:	InChI=1S/C5HF9O2/c6-3(7,8)1(4(9,10)11)16-2(15)5(12,13)14/h1H
InchiKey:	QFOKVELJLZLFMA-UHFFFAOYSA-N
Formula:	C5HF9O2
SMILES:	O=C(OC(C(F)(F)F)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]:	264.05
CAS:	42031-15-2

## Physical Properties

Property code	Value	Unit	Source
gf	-1989.91	kJ/mol	Joback Method
hf	-2187.85	kJ/mol	Joback Method
hfus	13.45	kJ/mol	Joback Method
hvap	24.25	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.585		Crippen Method
mvol	104.680	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
tb	373.39	K	Joback Method
tc	510.13	K	Joback Method
tf	215.84	K	Joback Method
vc	0.463	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.94	J/molxK	487.34	Joback Method
cpg	242.04	J/molxK	373.39	Joback Method
cpg	250.79	J/molxK	396.18	Joback Method
cpg	259.05	J/molxK	418.97	Joback Method
cpg	266.81	J/molxK	441.76	Joback Method
cpg	274.10	J/molxK	464.55	Joback Method
cpg	287.35	J/molxK	510.13	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=C42031152&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C42031152&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>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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