

# 3-Methyl-3-buten-1-ol, trifluoroacetate

**Inchi:** InChI=1S/C7H9F3O2/c1-5(2)3-4-12-6(11)7(8,9)10/h1,3-4H2,2H3  
**InchiKey:** IHPYFPWQBOSHJK-UHFFFAOYSA-N  
**Formula:** C7H9F3O2  
**SMILES:** C=C(C)CCOC(=O)C(F)(F)F  
**Mol. weight [g/mol]:** 182.14

## Physical Properties

Property code	Value	Unit	Source
gf	-728.16	kJ/mol	Joback Method
hf	-914.05	kJ/mol	Joback Method
hfus	15.91	kJ/mol	Joback Method
hvap	35.99	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.058		Crippen Method
mcvol	117.940	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinpol	914.60		NIST Webbook
tb	426.99	K	Joback Method
tc	593.90	K	Joback Method
tf	229.28	K	Joback Method
vc	0.476	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.10	J/molxK	426.99	Joback Method
cpg	260.37	J/molxK	454.81	Joback Method
cpg	270.14	J/molxK	482.63	Joback Method
cpg	279.45	J/molxK	510.44	Joback Method
cpg	288.29	J/molxK	538.26	Joback Method
cpg	296.69	J/molxK	566.08	Joback Method
cpg	304.67	J/molxK	593.90	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=U352293&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352293&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>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>rinpol:</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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