

# 4,4,4-Trifluoro-3-hydroxy-3-methylbutyric acid

<b>Inchi:</b>	InChI=1S/C5H7F3O3/c1-4(11,2-3(9)10)5(6,7)8/h11H,2H2,1H3,(H,9,10)
<b>InchiKey:</b>	JCJGOWYCFRASTM-UHFFFAOYSA-N
<b>Formula:</b>	C5H7F3O3
<b>SMILES:</b>	CC(O)(CC(=O)O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	172.10
<b>CAS:</b>	338-03-4

## Physical Properties

Property code	Value	Unit	Source
gf	-990.09	kJ/mol	Joback Method
hf	-1169.40	kJ/mol	Joback Method
hfus	12.89	kJ/mol	Joback Method
hvap	61.78	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	0.774		Crippen Method
mcvol	99.930	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
tb	543.38	K	Joback Method
tc	705.79	K	Joback Method
tf	324.29	K	Joback Method
vc	0.392	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.99	J/molxK	543.38	Joback Method
cpg	263.74	J/molxK	570.45	Joback Method
cpg	270.03	J/molxK	597.52	Joback Method
cpg	275.90	J/molxK	624.58	Joback Method
cpg	281.38	J/molxK	651.65	Joback Method
cpg	286.48	J/molxK	678.72	Joback Method
cpg	291.23	J/molxK	705.79	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.50 ± 1.50	K	0.07	NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C338034&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C338034&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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