

# «alpha»-Hydroxyisobutyric acid, trifluoroacetate

Inchi:	InChI=1S/C6H7F3O4/c1-5(2,3(10)11)13-4(12)6(7,8)9/h1-2H3,(H,10,11)
InchiKey:	KKKNBLWCXHRHFB-UHFFFAOYSA-N
Formula:	C6H7F3O4
SMILES:	CC(C)(OC(=O)C(F)(F)F)C(=O)O
Mol. weight [g/mol]:	200.11

## Physical Properties

Property code	Value	Unit	Source
gf	-1078.77	kJ/mol	Joback Method
hf	-1282.61	kJ/mol	Joback Method
hfus	14.18	kJ/mol	Joback Method
hvap	56.49	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	0.955		Crippen Method
mcvol	115.590	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpola	981.00		NIST Webbook
rinpola	981.00		NIST Webbook
tb	550.37	K	Joback Method
tc	725.25	K	Joback Method
tf	346.90	K	Joback Method
vc	0.453	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.55	J/mol×K	550.37	Joback Method
cpg	298.55	J/mol×K	579.52	Joback Method
cpg	306.03	J/mol×K	608.66	Joback Method
cpg	313.02	J/mol×K	637.81	Joback Method
cpg	319.54	J/mol×K	666.96	Joback Method
cpg	325.61	J/mol×K	696.10	Joback Method
cpg	331.26	J/mol×K	725.25	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=U374330&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374330&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>hvp:</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>rinp:</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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