

# 2-Hydroxyisocaproic acid, heptafluorobutyrate

<b>Inchi:</b>	InChI=1S/C10H11F7O4/c1-4(2)3-5(6(18)19)21-7(20)8(11,12)9(13,14)10(15,16)17/h4-5H
<b>InchiKey:</b>	GGSQFGBRSVUXHW-UHFFFAOYSA-N
<b>Formula:</b>	C10H11F7O4
<b>SMILES:</b>	CC(C)CC(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(=O)O
<b>Mol. weight [g/mol]:</b>	328.18

## Physical Properties

Property code	Value	Unit	Source
gf	-1826.37	kJ/mol	Joback Method
hf	-2168.92	kJ/mol	Joback Method
hfus	22.40	kJ/mol	Joback Method
hvap	60.05	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.862		Crippen Method
mcvol	179.030	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinqol	1200.00		NIST Webbook
tb	634.86	K	Joback Method
tc	795.77	K	Joback Method
tf	366.76	K	Joback Method
vc	0.726	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.88	J/molxK	634.86	Joback Method
cpg	523.80	J/molxK	661.68	Joback Method
cpg	533.09	J/molxK	688.50	Joback Method
cpg	541.77	J/molxK	715.32	Joback Method
cpg	549.87	J/molxK	742.14	Joback Method
cpg	557.44	J/molxK	768.95	Joback Method
cpg	564.50	J/molxK	795.77	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=U374894&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374894&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>hvac:</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>mccol:</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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