

# 4-Hydroxy-6-oxohept-4-enoic acid, pentafluoropropionate

<b>Inchi:</b>	InChI=1S/C10H9F5O5/c1-5(16)4-6(2-3-7(17)18)20-8(19)9(11,12)10(13,14)15/h4H,2-3H2
<b>InchiKey:</b>	OLVDGDKLKGAAHMM-XQRRVVYSFSA-N
<b>Formula:</b>	C10H9F5O5
<b>SMILES:</b>	CC(=O)C=C(CCC(=O)O)OC(=O)C(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	304.17

## Physical Properties

Property code	Value	Unit	Source
gf	-1491.96	kJ/mol	Joback Method
hf	-1762.54	kJ/mol	Joback Method
hfus	31.19	kJ/mol	Joback Method
hvap	70.54	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.065		Crippen Method
mcvol	172.760	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinqol	1278.00		NIST Webbook
tb	698.34	K	Joback Method
tc	873.66	K	Joback Method
tf	424.05	K	Joback Method
vc	0.700	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.99	J/molxK	698.34	Joback Method
cpg	491.35	J/molxK	727.56	Joback Method
cpg	499.14	J/molxK	756.78	Joback Method
cpg	506.39	J/molxK	786.00	Joback Method
cpg	513.15	J/molxK	815.22	Joback Method
cpg	519.45	J/molxK	844.44	Joback Method
cpg	525.34	J/molxK	873.66	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=U374241&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374241&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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