

# 3-Hexanol, heptafluorobutyrate

<b>Inchi:</b>	InChI=1S/C10H13F7O2/c1-3-5-6(4-2)19-7(18)8(11,12)9(13,14)10(15,16)17/h6H,3-5H2,1
<b>InchiKey:</b>	GTDOABUUMNBOTM-UHFFFAOYSA-N
<b>Formula:</b>	C10H13F7O2
<b>SMILES:</b>	CCCC(CC)OC(=O)C(F)(F)C(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	298.20

## Physical Properties

Property code	Value	Unit	Source
gf	-1558.19	kJ/mol	Joback Method
hf	-1898.83	kJ/mol	Joback Method
hfus	20.24	kJ/mol	Joback Method
hvap	37.02	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.941		Crippen Method
mvol	171.590	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	860.00		NIST Webbook
rinpol	860.00		NIST Webbook
tb	489.25	K	Joback Method
tc	639.92	K	Joback Method
tf	271.01	K	Joback Method
vc	0.707	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.04	J/mol×K	489.25	Joback Method
cpg	447.25	J/mol×K	514.36	Joback Method
cpg	459.76	J/mol×K	539.47	Joback Method
cpg	471.59	J/mol×K	564.59	Joback Method
cpg	482.76	J/mol×K	589.70	Joback Method
cpg	493.30	J/mol×K	614.81	Joback Method
cpg	503.25	J/mol×K	639.92	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U352367&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352367&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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>

# 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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