

# 3-Methyl-2-buten-1-ol, heptafluorobutyrate

<b>Inchi:</b>	InChI=1S/C9H9F7O2/c1-5(2)3-4-18-6(17)7(10,11)8(12,13)9(14,15)16/h3H,4H2,1-2H3
<b>InchiKey:</b>	BQWPOYIWRJFRHC-UHFFFAOYSA-N
<b>Formula:</b>	C9H9F7O2
<b>SMILES:</b>	CC(C)=CCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	282.16

## Physical Properties

Property code	Value	Unit	Source
gf	-1492.50	kJ/mol	Joback Method
hf	-1765.48	kJ/mol	Joback Method
hfus	20.06	kJ/mol	Joback Method
hvap	35.22	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.329		Crippen Method
mcvol	153.200	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpola	833.10		NIST Webbook
tb	470.85	K	Joback Method
tc	627.68	K	Joback Method
tf	255.70	K	Joback Method
vc	0.637	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.09	J/molxK	470.85	Joback Method
cpg	384.25	J/molxK	496.99	Joback Method
cpg	395.66	J/molxK	523.13	Joback Method
cpg	406.35	J/molxK	549.27	Joback Method
cpg	416.35	J/molxK	575.41	Joback Method
cpg	425.72	J/molxK	601.54	Joback Method
cpg	434.47	J/molxK	627.68	Joback Method

# Sources

<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=U352700&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352700&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>
<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>

# 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>mccvol:</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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