

# Butanoic acid, heptafluoro-, 2-propenyl ester

<b>Other names:</b>	Heptafluorobutyric acid, 2-propenyl ester Allyl 2,2,3,3,4,4,4-heptafluorobutanoate Allyl alcohol, heptafluorobutyrate Allyl heptafluorobutyrate Allyl perfluorobutyrate Butyric acid, heptafluoro-, allyl ester
<b>Inchi:</b>	InChI=1S/C7H5F7O2/c1-2-3-16-4(15)5(8,9)6(10,11)7(12,13)14/h2H,1,3H2
<b>InchiKey:</b>	JFBHYYDXTQBWAL-UHFFFAOYSA-N
<b>Formula:</b>	C7H5F7O2
<b>SMILES:</b>	C=CCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	254.10
<b>CAS:</b>	17165-55-8

## Physical Properties

Property code	Value	Unit	Source
gf	-1493.17	kJ/mol	Joback Method
hf	-1706.20	kJ/mol	Joback Method
hfus	14.71	kJ/mol	Joback Method
hvap	30.06	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.549		Crippen Method
mcvol	125.020	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpola	724.10		NIST Webbook
tb	417.73	K	Joback Method
tc	568.69	K	Joback Method
tf	250.44	K	Joback Method
vc	0.525	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.52	J/mol×K	417.73	Joback Method
cpg	297.98	J/mol×K	442.89	Joback Method

cpg	307.80	J/mol×K	468.05	Joback Method
cpg	317.00	J/mol×K	493.21	Joback Method
cpg	325.61	J/mol×K	518.37	Joback Method
cpg	333.66	J/mol×K	543.53	Joback Method
cpg	341.18	J/mol×K	568.69	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C17165558&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17165558&amp;Units=SI</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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