

# 1,3-Butadiene, 1,1,2,3,4,4-hexafluoro-

<b>Other names:</b>	Hexafluoro-1,3-butadiene Perfluoro-1,3-butadiene 1,1,2,3,4,4-Hexafluoro-1,3-butadiene CF <sub>2</sub> =CFCF=CF <sub>2</sub> Perfluorobutadiene-1,3 Hexafluorobutadiene-1,3 1,1,2,3,4,4-hexafluorobuta-1,3-diene
<b>Inchi:</b>	InChI=1S/C4F6/c5-1(3(7)8)2(6)4(9)10
<b>InchiKey:</b>	LGPPATCNSOSOQH-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>4</sub> F <sub>6</sub>
<b>SMILES:</b>	FC(F)=C(F)C(F)=C(F)F
<b>Mol. weight [g/mol]:</b>	162.03
<b>CAS:</b>	685-63-2

## Physical Properties

Property code	Value	Unit	Source
gf	-1059.82	kJ/mol	Joback Method
hf	-942.20	kJ/mol	NIST Webbook
hfus	19.76	kJ/mol	Joback Method
hvap	19.83	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
log10ws	-3.30		Crippen Method
logp	3.142		Crippen Method
mcvol	69.240	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
tb	279.50 ± 0.50	K	NIST Webbook
tc	432.55	K	Joback Method
vc	0.332	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.21	J/mol×K	409.52	Joback Method
cpg	117.90	J/mol×K	294.38	Joback Method

cpg	123.78	J/mol×K	317.41	Joback Method
cpg	129.34	J/mol×K	340.44	Joback Method
cpg	134.59	J/mol×K	363.46	Joback Method
cpg	139.55	J/mol×K	386.49	Joback Method
cpg	148.61	J/mol×K	432.55	Joback Method
hvapt	25.90	kJ/mol	308.00	NIST Webbook

## 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=C685632&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C685632&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>vc:</b>	Critical Volume

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