Butanal, heptafluoro-

Other names:	Butyraldehyde, heptafluoro-
	Heptafluorobutyraldehyde
	Perfluorobutyraldehyde
	Heptafluoro-n-butyraldehyde
Inchi:	InChI=1S/C4HF7O/c5-2(6,1-12)3(7,8)4(9,10)11/h1H
InchiKey:	IQJZGNJYXIIMGP-UHFFFAOYSA-N
Formula:	C4HF7O
SMILES:	O=CC(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	198.04
CAS:	375-02-0

Physical Properties

Property code	Value	Unit	Source
gf	-1471.87	kJ/mol	Joback Method
hf	-1610.49	kJ/mol	Joback Method
hfus	7.72	kJ/mol	Joback Method
hvap	21.61	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.018		Crippen Method
mcvol	81.180	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
tb	368.50 ± 0.50	K	NIST Webbook
tb	302.00 ± 4.00	K	NIST Webbook
tc	466.28	K	Joback Method
tf	188.23	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.37	J/mol×K	324.78	Joback Method
cpg	178.01	J/mol×K	348.36	Joback Method
cpg	186.09	J/mol×K	371.95	Joback Method
cpg	193.61	J/mol×K	395.53	Joback Method

cpg	200.61	J/mol×K	419.11	Joback Method
cpg	207.10	J/mol×K	442.70	Joback Method
cpg	213.12	J/mol×K	466.28	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C375020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume