2-Butene, 2-chloro-1,1,1,4,4,4-hexafluoro-

Other names:	2-Chloro-1,1,1,4,4,4-hexafluorobutene-2
	CHFB
	1,1,1,4,4,4-Hexafluoro-2-chloro-2-butene
	1,1,1,4,4,4-Hexafluoro-2-chlorobut-2-ene
	2-Chloro-1,1,1,4,4,4-hexafluoro-2-butene
Inchi:	InChI=1S/C4HClF6/c5-2(4(9,10)11)1-3(6,7)8/h1H/b2-1-
InchiKey:	JRENXZBKMHPULY-UPHRSURJSA-N
Formula:	C4HClF6
SMILES:	FC(F)(F)C=C(Cl)C(F)(F)F
Mol. weight [g/mol]:	198.49
CAS:	400-44-2

Physical Properties

Property code	Value	Unit	Source
gf	-1120.64	kJ/mol	Joback Method
hf	-1228.36	kJ/mol	Joback Method
hfus	12.86	kJ/mol	Joback Method
hvap	21.43	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.234		Crippen Method
mcvol	85.780	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
tb	306.50 ± 0.50	K	NIST Webbook
tc	471.60	K	Joback Method
tf	154.10	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.83	J/mol×K	321.55	Joback Method
cpg	162.03	J/mol×K	346.56	Joback Method
cpg	169.66	J/mol×K	371.57	Joback Method
cpg	176.74	J/mol×K	396.58	Joback Method

cpg	183.30	J/mol×K	421.59	Joback Method
cpg	189.36	J/mol×K	446.59	Joback Method
cpg	194.94	J/mol×K	471.60	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=C400442&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