Octafluoro-2-butene

Other names:	1,1,1,2,3,4,4,4-octafluorobut-2-ene
	2-Butene, 1,1,1,2,3,4,4,4-octafluoro-
	2-Butene, octafluoro-
	FC-1318
	NA 2422
	Octafluorobut-2-ene
	Octafluorobutene-2
	Perfluoro-1-methylpropene
	Perfluoro-2-butene
	Perfluorobut-2-ene
	Perfluorobutene-2
	R 1318my
	UN 2422
Inchi:	InChI=1S/C4F8/c5-1(3(7,8)9)2(6)4(10,11)12
InchiKey:	WSJULBMCKQTTIG-UHFFFAOYSA-N
Formula:	C4F8
SMILES:	FC(=C(F)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]:	200.03
CAS:	360-89-4

Physical Properties

Property code	Value	Unit	Source
gf	-1506.88	kJ/mol	Joback Method
hf	-1614.63	kJ/mol	Joback Method
hfus	13.51	kJ/mol	Joback Method
hvap	15.49	kJ/mol	Joback Method
ie	11.25	eV	NIST Webbook
log10ws	-3.37		Crippen Method
logp	3.262		Crippen Method
mcvol	77.080	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
tb	274.30	K	NIST Webbook
tc	409.82	K	Joback Method
tf	111.40	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.06	J/mol×K	282.54	Joback Method
cpg	151.05	J/mol×K	303.75	Joback Method
cpg	158.59	J/mol×K	324.97	Joback Method
cpg	165.70	J/mol×K	346.18	Joback Method
cpg	172.38	J/mol×K	367.39	Joback Method
cpg	178.65	J/mol×K	388.60	Joback Method
cpg	184.53	J/mol×K	409.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.91458e+01
Coeff. B	-4.35218e+03
Coeff. C	-6.97575e+00
Coeff. D	8.81174e-06
Temperature range (K), min.	138.15
Temperature range (K), max.	392.00

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=C360894&Units=SI

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1744

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume