2-Propanone, 1,1,1,3,3,3-hexafluoro-

Other names:	(CF3)2CO
	1,1,1,3,3,3-Hexafluoro-2-propanone
	2-Propanone, hexafluoro-
	6FK
	Acetone, hexafluoro-
	GC 7887
	HEXAFLUOROACETONE
	Hexafluoropropanone
	NCI-C56440
	NSC 202438
	PERFLUOROACETONE
	Perfluoro-2-propanone
	UN 2420
Inchi:	InChI=1S/C3F6O/c4-2(5,6)1(10)3(7,8)9
InchiKey:	VBZWSGALLODQNC-UHFFFAOYSA-N
Formula:	C3F6O
SMILES:	O=C(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]:	166.02
CAS:	684-16-2

Physical Properties

Property code	Value	Unit	Source
af	0.3650		KDB
affp	670.40	kJ/mol	NIST Webbook
basg	639.70	kJ/mol	NIST Webbook
ea	0.44	eV	NIST Webbook
gf	-1317.72	kJ/mol	Joback Method
hf	-1411.99	kJ/mol	Joback Method
hfus	8.78	kJ/mol	Joback Method
hvap	21.52	kJ/mol	Joback Method
ie	11.68	eV	NIST Webbook
ie	11.44	eV	NIST Webbook
ie	11.57 ± 0.13	eV	NIST Webbook
ie	12.09 ± 0.02	eV	NIST Webbook
log10ws	-1.68		Crippen Method
logp	1.680		Crippen Method
mcvol	65.320	ml/mol	McGowan Method

pc	2840.00	kPa	KDB
pc	2832.00 ± 3.44	kPa	NIST Webbook
rhoc	504.71 ± 5.05	kg/m3	NIST Webbook
sl	286.60	J/mol×K	NIST Webbook
tb	247.20	K	NIST Webbook
tb	245.70	K	NIST Webbook
tb	245.20	K	NIST Webbook
tb	245.70	K	KDB
tc	357.14 ± 0.20	K	NIST Webbook
tc	357.14	K	KDB
tf	148.00	K	KDB
tt	147.70 ± 0.02	K	NIST Webbook
vc	0.329	m3/kmol	KDB
zc	0.3146580		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.11	J/mol×K	454.82	Joback Method
cpg	134.60	J/mol×K	335.03	Joback Method
cpg	140.89	J/mol×K	358.99	Joback Method
cpg	146.77	J/mol×K	382.94	Joback Method
cpg	152.25	J/mol×K	406.90	Joback Method
cpg	157.36	J/mol×K	430.86	Joback Method
cpg	127.89	J/mol×K	311.07	Joback Method
cpl	181.29	J/mol×K	245.00	NIST Webbook
hfust	8.38	kJ/mol	147.70	NIST Webbook
hfust	8.38	kJ/mol	147.70	NIST Webbook
hvapt	21.61	kJ/mol	245.87	NIST Webbook
sfust	56.75	J/mol×K	147.70	NIST Webbook
svapt	87.91	J/mol×K	245.87	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42172e+01

Coeff. B	-2.00849e+03
Coeff. C	-3.66370e+01
Temperature range (K), min.	180.83
Temperature range (K), max.	357.14

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1783.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C684162&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
rhoc:	Critical density
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions

svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility