2,4-Pentanedione, 1,1,1-trifluoro-

Other names:	(Trifluoroacetyl)acetone
	1,1,1-Trifluoro-2,4-pentanedione
	1,1,1-Trifluoroacetylacetone
	CF3COH=CHCOCH3
	1,1,1-Trifluoro-2,4-pentadione
	Acetyl trifluoroacetone
	1,1,1-trifluoropentane-2,4-dione
Inchi:	InChI=1S/C5H5F3O2/c1-3(9)2-4(10)5(6,7)8/h2H2,1H3
InchiKey:	SHXHPUAKLCCLDV-UHFFFAOYSA-N
Formula:	C5H5F3O2
SMILES:	CC(=O)CC(=O)C(F)(F)F
Mol. weight [g/mol]:	154.09
CAS:	367-57-7

Physical Properties

Property code	Value	Unit	Source
chl	-2179.90 ± 2.60	kJ/mol	NIST Webbook
gf	-848.21	kJ/mol	Joback Method
hf	-1003.30 ± 3.30	kJ/mol	NIST Webbook
hf	-993.30 ± 3.40	kJ/mol	NIST Webbook
hfl	-1040.20 ± 3.30	kJ/mol	NIST Webbook
hfus	13.73	kJ/mol	Joback Method
hvap	37.27	kJ/mol	NIST Webbook
hvap	37.20 ± 0.20	kJ/mol	NIST Webbook
ie	9.80 ± 0.10	eV	NIST Webbook
ie	9.47	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	9.92 ± 0.07	eV	NIST Webbook
log10ws	-1.14		Crippen Method
logp	1.097		Crippen Method
mcvol	89.760	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
tb	380.20	K	NIST Webbook
tb	380.00	K	NIST Webbook
tb	379.20	K	NIST Webbook
tb	380.00	K	NIST Webbook
tc	589.75	K	Joback Method

tf	250.16	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.68	J/mol×K	416.12	Joback Method
cpg	191.74	J/mol×K	445.06	Joback Method
cpg	199.34	J/mol×K	474.00	Joback Method
cpg	206.49	J/mol×K	502.94	Joback Method
cpg	213.23	J/mol×K	531.88	Joback Method
cpg	219.56	J/mol×K	560.81	Joback Method
cpg	225.50	J/mol×K	589.75	Joback Method
hvapt	31.21	kJ/mol	380.20	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C367577&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume