2,4-Pentanedione, 1,1,1,5,5,5-hexafluoro-

Other names:	1,1,1,5,5,5-Hexafluoro-2,4-pentanedione
	1,1,1,5,5,5-Hexafluoroacetylacetone
	1,1,1,5,5,5-hexafluoropentane-2,4-dione
	1,3-Bis(trifluoromethyl)propane-1,3-dione
	HEXAFLUORO-2,4-PENTANEDIONE
	Hexafluoroacetylacetone
Inchi:	InChI=1S/C5H2F6O2/c6-4(7,8)2(12)1-3(13)5(9,10)11/h1H2
InchiKey:	QAMFBRUWYYMMGJ-UHFFFAOYSA-N
Formula:	C5H2F6O2
SMILES:	O=C(CC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]:	208.06
CAS:	1522-22-1

Physical Properties

Property code	Value	Unit	Source
af	0.2780		KDB
gf	-1429.80	kJ/mol	Joback Method
hf	-1565.85	kJ/mol	Joback Method
hfus	15.56	kJ/mol	Joback Method
hvap	30.66	kJ/mol	NIST Webbook
hvap	30.60 ± 0.10	kJ/mol	NIST Webbook
ie	10.74 ± 0.07	eV	NIST Webbook
ie	10.55 ± 0.05	eV	NIST Webbook
log10ws	-1.80		Crippen Method
logp	1.639		Crippen Method
mcvol	95.070	ml/mol	McGowan Method
pc	2867.16 ± 8.00	kPa	NIST Webbook
pc	2767.00	kPa	KDB
rinpol	526.00		NIST Webbook
tb	343.00	K	NIST Webbook
tb	343.20	K	NIST Webbook
tb	343.20	K	NIST Webbook
tb	343.00	K	NIST Webbook
tb	327.30	K	KDB
tc	485.10	K	KDB
tc	485.10 ± 1.00	K	NIST Webbook
tf	254.35	K	Joback Method

vc	0.290 ± 0.008	m3/kmol	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.90	J/mol×K	516.03	Joback Method
cpg	245.93	J/mol×K	542.36	Joback Method
cpg	210.99	J/mol×K	410.70	Joback Method
cpg	218.98	J/mol×K	437.03	Joback Method
cpg	226.45	J/mol×K	463.36	Joback Method
cpg	233.42	J/mol×K	489.69	Joback Method
cpg	251.51	J/mol×K	568.69	Joback Method
hvapt	27.05	kJ/mol	343.20	NIST Webbook
hvapt	33.10	kJ/mol	301.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1522221&Units=SI
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/mol1788.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume