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

Physical Properties

Property code	Value	Unit	Source
af	0.2780		KDB
hf	-1593.63	kJ/mol	Cheméo Relay (1.0)
hfus	15.56	kJ/mol	Joback Method
hvap	30.60 ± 0.10	kJ/mol	NIST Webbook
hvap	30.66	kJ/mol	NIST Webbook
ie	10.74 ± 0.07	eV	NIST Webbook
ie	10.55 ± 0.05	eV	NIST Webbook
logp	1.639		Crippen Method
mcvol	95.070	ml/mol	McGowan Method
pc	2767.00	kPa	KDB
pc	2867.16 ± 8.00	kPa	NIST Webbook
rinpol	526.00		NIST Webbook
tb	327.30	K	KDB
tb	343.00	K	NIST Webbook
tb	343.20	K	NIST Webbook
tb	343.20	K	NIST Webbook
tb	343.00	K	NIST Webbook
tc	485.10 ± 1.00	K	NIST Webbook
tc	485.10	K	KDB
tf	281.13	K	Cheméo Relay (1.0)
vc	0.290 ± 0.008	m3/kmol	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	239.90	J/mol×K	516.03	Joback Method
cpg	245.93	J/mol×K	542.36	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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1788

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1522221&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
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
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