Benzoic acid, pentafluoro-

Other names:	Pentafluorobenzoic acid
	Perfluorobenzoic acid
	2,3,4,5,6-Pentafluorobenzoic acid
Inchi:	InChI=1S/C7HF5O2/c8-2-1(7(13)14)3(9)5(11)6(12)4(2)10/h(H,13,14)
InchiKey:	YZERDTREOUSUHF-UHFFFAOYSA-N
Formula:	C7HF5O2
SMILES:	O=C(O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	212.07
CAS:	602-94-8

Physical Properties

Property code	Value	Unit	Source
chs	-2552.80 ± 1.00	kJ/mol	NIST Webbook
gf	-1167.47	kJ/mol	Joback Method
hf	-1148.40 ± 1.00	kJ/mol	NIST Webbook
hfs	-1239.90 ± 1.00	kJ/mol	NIST Webbook
hfus	27.07	kJ/mol	Joback Method
hsub	91.50 ± 0.40	kJ/mol	NIST Webbook
hvap	56.10	kJ/mol	Joback Method
ie	10.20	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-3.19		Crippen Method
logp	2.080		Crippen Method
mcvol	102.020	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
tb	493.20	K	NIST Webbook
tb	493.00	K	NIST Webbook
tc	724.23	K	Joback Method
tf	371.37	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.42	J/mol×K	553.54	Joback Method
cpg	235.90	J/mol×K	581.99	Joback Method
cpg	241.15	J/mol×K	610.44	Joback Method
cpg	246.16	J/mol×K	638.88	Joback Method
cpg	250.95	J/mol×K	667.33	Joback Method
cpg	255.50	J/mol×K	695.78	Joback Method
cpg	259.82	J/mol×K	724.23	Joback Method
hsubt	91.60 ± 4.20	kJ/mol	347.00	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=C602948&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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

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