Benzoic acid, 4-fluoro-

Other names:	4-Fluorobenzoic acid
	Benzoic acid, p-fluoro-
	p-Fluorobenzoic acid
	para-Fluorobenzoic acid
Inchi:	InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
InchiKey:	BBYDXOIZLAWGSL-UHFFFAOYSA-N
Formula:	C7H5FO2
SMILES:	O=C(O)c1ccc(F)cc1
Mol. weight [g/mol]:	140.11
CAS:	456-22-4

Physical Properties

Property code	Value	Unit	Source
chs	-3063.20 ± 0.88	kJ/mol	NIST Webbook
chs	-3094.70	kJ/mol	NIST Webbook
chs	-3063.80 ± 0.80	kJ/mol	NIST Webbook
chs	-3061.50 ± 1.20	kJ/mol	NIST Webbook
gf	-349.71	kJ/mol	Joback Method
hf	-423.67	kJ/mol	Joback Method
hfs	-584.90	kJ/mol	NIST Webbook
hfs	-586.80 ± 1.60	kJ/mol	NIST Webbook
hfs	-584.70 ± 0.90	kJ/mol	NIST Webbook
hfus	16.31	kJ/mol	Joback Method
hsub	93.10 ± 3.80	kJ/mol	NIST Webbook
hsub	91.30 ± 3.00	kJ/mol	NIST Webbook
hvap	56.72	kJ/mol	Joback Method
ie	9.90 ± 0.20	eV	NIST Webbook
log10ws	-2.07		Aqueous Solubility Prediction Method
logp	1.524		Crippen Method
mcvol	94.940	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
tb	536.54	K	Joback Method
tc	736.94	K	Joback Method
tf	456.10	K	Thermochemistry of halogenobenzoic acids as an access to PC-SAFT solubility modeling

vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.46	J/mol×K	536.54	Joback Method
cpg	209.29	J/mol×K	569.94	Joback Method
cpg	216.64	J/mol×K	603.34	Joback Method
cpg	223.53	J/mol×K	636.74	Joback Method
cpg	229.98	J/mol×K	670.14	Joback Method
cpg	236.00	J/mol×K	703.54	Joback Method
cpg	241.62	J/mol×K	736.94	Joback Method
hfust	20.90	kJ/mol	451.20	NIST Webbook
hsubt	91.20 ± 1.30	kJ/mol	370.00	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C456224&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermochemistry of halogenobenzoic acids as an access to PC-SAFT solubility modeling:	https://www.doi.org/10.1016/j.fluid.2015.10.001
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume