P-fluorobenzenesulfonic acid

Other names: 4-fluorobenzenesulphonic acid
Inchi: InChI=1S/C6H5FO3S/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,(H,8,9,10)
InchiKey: WVSYONICNIDYBE-UHFFFAOYSA-N
Formula: C6H5FO3S
SMILES: O=S(=O)(O)c1ccc(F)cc1
Mol. weight [g/mol]: 176.17
CAS: 368-88-7

Physical Properties

Property code	Value	Unit	Source
gf	-697.75	kJ/mol	Joback Method
hf	-743.80	kJ/mol	Joback Method
hfus	23.49	kJ/mol	Joback Method
hvap	66.39	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.072		Crippen Method
mcvol	107.370	ml/mol	McGowan Method
pc	6141.84	kPa	Joback Method
tb	507.57	K	Joback Method
tc	695.73	K	Joback Method
tf	296.29	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.56	J/mol×K	507.57	Joback Method
cpg	229.90	J/mol×K	538.93	Joback Method
cpg	237.80	J/mol×K	570.29	Joback Method
cpg	245.25	J/mol×K	601.65	Joback Method
cpg	252.26	J/mol×K	633.01	Joback Method
cpg	258.83	J/mol×K	664.37	Joback Method
cpg	264.96	J/mol×K	695.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C368887&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

Legend

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
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