2,3,5,6-Tetrafluorophenol

Other names: Phenol, 2,3,5,6-tetrafluoro-
Inchi: InChI=1S/C6H2F4O/c7-2-1-3(8)5(10)6(11)4(2)9/h1,11H
InchiKey: PBYIIRLNRCVTMQ-UHFFFAOYSA-N
Formula: C6H2F4O
SMILES: Oc1c(F)c(F)cc(F)c1F
Mol. weight [g/mol]: 166.07
CAS: 769-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-850.70	kJ/mol	Joback Method
hf	-926.80	kJ/mol	Joback Method
hfus	22.27	kJ/mol	Joback Method
hvap	42.96	kJ/mol	Joback Method
ie	9.40 ± 0.02	eV	NIST Webbook
log10ws	-2.35		Crippen Method
logp	1.949		Crippen Method
mcvol	84.590	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	413.20	K	NIST Webbook
tb	415.00	K	NIST Webbook
tc	646.82	K	Joback Method
tf	335.44	K	Joback Method
vc	0.301	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.42	J/mol×K	456.00	Joback Method
cpg	185.79	J/mol×K	487.80	Joback Method
cpg	191.74	J/mol×K	519.61	Joback Method
cpg	197.29	J/mol×K	551.41	Joback Method
cpg	202.48	J/mol×K	583.22	Joback Method
cpg	207.34	J/mol×K	615.02	Joback Method

cpg	211.90	J/mol×K	646.82	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C769391&Units=SI

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
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