5-Fluoro-2-hydroxyacetophenone

Other names:	2-Hydroxy-5-fluoroacetophenone
	5'-Fluoro-2'-hydroxyacetophenone
	Ethanone, 1-(5-fluoro-2-hydroxyphenyl)-
	1-(5-fluoro-2-hydroxyphenyl)ethan-1-one
Inchi:	InChI=1S/C8H7FO2/c1-5(10)7-4-6(9)2-3-8(7)11/h2-4,11H,1H3
InchiKey:	KOFFXZYMDLWRHX-UHFFFAOYSA-N
Formula:	C8H7FO2
SMILES:	CC(=O)c1cc(F)ccc1O
Mol. weight [g/mol]:	154.14
CAS:	394-32-1

Physical Properties

Property code	Value	Unit	Source
gf	-359.09	kJ/mol	Joback Method
hf	-469.39	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	55.28	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.734		Crippen Method
mcvol	109.030	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
tb	547.86	K	Joback Method
tc	772.34	K	Joback Method
tf	381.10	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.26	J/mol×K	547.86	Joback Method
cpg	254.87	J/mol×K	585.27	Joback Method
cpg	263.76	J/mol×K	622.69	Joback Method
cpg	272.02	J/mol×K	660.10	Joback Method
cpg	279.70	J/mol×K	697.51	Joback Method

cpg	286.87	J/mol×K	734.92	Joback Method
cpg	293.61	J/mol×K	772.34	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=C394321&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
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