Ethanone, 1-(4-fluorophenyl)-

Other names:	Acetophenone, 4'-fluoro- p-Fluoroacetophenone 4-Fluoroacetophenone 4'-Fluoroacetophenone para-Fluoroacetophenone
Inchi:	InChI=1S/C8H7FO/c1-6(10)7-2-4-8(9)5-3-7/h2-5H,1H3
InchiKey:	ZDPAWHACYDRYIW-UHFFFAOYSA-N
Formula:	C8H7FO
SMILES:	CC(=O)c1ccc(F)cc1
Mol. weight [g/mol]:	138.14
CAS:	403-42-9

Physical Properties

Property code	Value	Unit	Source
affp	858.60	kJ/mol	NIST Webbook
basg	826.80	kJ/mol	NIST Webbook
ea	0.40 ± 0.01	eV	NIST Webbook
gf	-204.47	kJ/mol	Joback Method
hf	-292.08	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	42.27	kJ/mol	Joback Method
ie	9.60 ± 0.20	eV	NIST Webbook
log10ws	-2.46		Crippen Method
logp	2.028		Crippen Method
mcvol	103.160	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
rinpol	1029.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1040.70		NIST Webbook
rinpol	1029.70		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1047.60		NIST Webbook
tb	469.20	K	NIST Webbook
tc	678.42	K	Joback Method
tf	269.38	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.90	J/mol×K	467.24	Joback Method
cpg	211.62	J/mol×K	502.44	Joback Method
cpg	221.72	J/mol×K	537.63	Joback Method
cpg	231.22	J/mol×K	572.83	Joback Method
cpg	240.13	J/mol×K	608.03	Joback Method
cpg	248.49	J/mol×K	643.23	Joback Method
cpg	256.32	J/mol×K	678.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C403429&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

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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

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

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