Ethanone, 1-(3-fluorophenyl)-

Other names: Acetophenone, 3'-fluoro-
m-Fluoroacetophenone
3-Fluoroacetophenone
3'-Fluoroacetophenone
Inchi: InChI=1S/C8H7FO/c1-6(10)7-3-2-4-8(9)5-7/h2-5H,1H3
InchiKey: HCEKGPAHZCYRBZ-UHFFFAOYSA-N
Formula: C8H7FO
SMILES: CC(=O)c1cccc(F)c1
Mol. weight [g/mol]: 138.14
CAS: 455-36-7

Physical Properties

Property code	Value	Unit	Source
affp	845.70	kJ/mol	NIST Webbook
basg	813.80	kJ/mol	NIST Webbook
ea	0.58 ± 0.03	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	9.80 ± 0.10	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
tb	467.24	K	Joback Method
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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.20	K	1.00	NIST Webbook

Sources

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=C455367&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume