1-Butanone, 1-(4-fluorophenyl)-

Other names:	Butyrophenone, 4'-fluoro- p-Fluorobutyrophenone 4'-Fluorobutyrophenone 1-(4-Fluorophenyl)-1-butanone
Inchi:	InChI=1S/C10H11FO/c1-2-3-10(12)8-4-6-9(11)7-5-8/h4-7H,2-3H2,1H3
InchiKey:	QHDXPJMOWRLLRV-UHFFFAOYSA-N
Formula:	C10H11FO
SMILES:	CCCC(=O)c1ccc(F)cc1
Mol. weight [g/mol]:	166.19
CAS:	582-83-2

Physical Properties

Property code	Value	Unit	Source
gf	-187.63	kJ/mol	Joback Method
hf	-333.36	kJ/mol	Joback Method
hfus	19.99	kJ/mol	Joback Method
hvap	46.72	kJ/mol	Joback Method
ie	9.10 ± 0.20	eV	NIST Webbook
log10ws	-3.30		Crippen Method
logp	2.808		Crippen Method
mcvol	131.340	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	513.00	K	Joback Method
tc	718.14	K	Joback Method
tf	291.92	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.95	J/mol×K	513.00	Joback Method
cpg	297.83	J/mol×K	547.19	Joback Method
cpg	309.98	J/mol×K	581.38	Joback Method
cpg	321.44	J/mol×K	615.57	Joback Method

cpg	332.22	J/mol×K	649.76	Joback Method
cpg	342.35	J/mol×K	683.95	Joback Method
cpg	351.86	J/mol×K	718.14	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=C582832&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