4-Fluoro-2-methoxyacetophenone

Inchi: InChI=1S/C9H9FO2/c1-6(11)8-4-3-7(10)5-9(8)12-2/h3-5H,1-2H3
InchiKey: YOXBPWVWNQROBJ-UHFFFAOYSA-N
Formula: C9H9FO2
SMILES: COc1cc(F)ccc1C(C)=O
Mol. weight [g/mol]: 168.16
CAS: 51788-80-8

Physical Properties

Property code	Value	Unit	Source
gf	-310.68	kJ/mol	Joback Method
hf	-456.41	kJ/mol	Joback Method
hfus	18.20	kJ/mol	Joback Method
hvap	47.57	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.037		Crippen Method
mcvol	123.120	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	517.52	K	Joback Method
tc	724.99	K	Joback Method
tf	315.40	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.31	J/mol×K	517.52	Joback Method
cpg	275.58	J/mol×K	552.10	Joback Method
cpg	286.31	J/mol×K	586.68	Joback Method
cpg	296.50	J/mol×K	621.26	Joback Method
cpg	306.15	J/mol×K	655.83	Joback Method
cpg	315.26	J/mol×K	690.41	Joback Method
cpg	323.85	J/mol×K	724.99	Joback Method

Sources

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=C51788808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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