4'-Fluorovalerophenone

Other names: 4-Fluorovalerophenone
Inchi: InChI=1S/C11H13FO/c1-2-3-4-11(13)9-5-7-10(12)8-6-9/h5-8H,2-4H2,1H3
InchiKey: HBJRRAMFTUDWMQ-UHFFFAOYSA-N
Formula: C11H13FO
SMILES: CCCCC(=O)c1ccc(F)cc1
Mol. weight [g/mol]: 180.22
CAS: 29114-66-7

Physical Properties

Property code	Value	Unit	Source
gf	-179.21	kJ/mol	Joback Method
hf	-354.00	kJ/mol	Joback Method
hfus	22.58	kJ/mol	Joback Method
hvap	48.95	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.199		Crippen Method
mcvol	145.430	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
tb	535.88	K	Joback Method
tc	738.04	K	Joback Method
tf	303.19	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.86	J/mol×K	535.88	Joback Method
cpg	343.61	J/mol×K	569.57	Joback Method
cpg	356.61	J/mol×K	603.27	Joback Method
cpg	368.86	J/mol×K	636.96	Joback Method
cpg	380.41	J/mol×K	670.65	Joback Method
cpg	391.27	J/mol×K	704.35	Joback Method
cpg	401.47	J/mol×K	738.04	Joback Method

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=C29114667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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