2-Fluoro-4-(trifluoromethyl)acetophenone

Inchi: InChI=1S/C9H6F4O/c1-5(14)7-3-2-6(4-8(7)10)9(11,12)13/h2-4H,1H3
InchiKey: OLDXVWXLMGJVPH-UHFFFAOYSA-N
Formula: C9H6F4O
SMILES: CC(=O)c1ccc(C(F)(F)F)cc1F
Mol. weight [g/mol]: 206.14
CAS: 122023-29-4

Physical Properties

Property code	Value	Unit	Source
gf	-787.27	kJ/mol	Joback Method
hf	-921.27	kJ/mol	Joback Method
hfus	18.83	kJ/mol	Joback Method
hvap	41.41	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.047		Crippen Method
mcvol	122.560	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
tb	489.68	K	Joback Method
tc	680.50	K	Joback Method
tf	297.36	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.25	J/mol×K	489.68	Joback Method
cpg	281.00	J/mol×K	521.48	Joback Method
cpg	291.07	J/mol×K	553.29	Joback Method
cpg	300.50	J/mol×K	585.09	Joback Method
cpg	309.30	J/mol×K	616.89	Joback Method
cpg	317.52	J/mol×K	648.70	Joback Method
cpg	325.17	J/mol×K	680.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122023294&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

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