3-Fluorophenylacetone

Inchi: InChI=1S/C9H9FO/c1-7(11)5-8-3-2-4-9(10)6-8/h2-4,6H,5H2,1H3
InchiKey: UWCPYXSRCQVABG-UHFFFAOYSA-N
Formula: C9H9FO
SMILES: CC(=O)Cc1cccc(F)c1
Mol. weight [g/mol]: 152.17
CAS: 1737-19-5

Physical Properties

Property code	Value	Unit	Source
gf	-196.05	kJ/mol	Joback Method
hf	-312.72	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	44.50	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.957		Crippen Method
mcvol	117.250	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
tb	490.12	K	Joback Method
tc	698.29	K	Joback Method
tf	280.65	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.93	J/mol×K	490.12	Joback Method
cpg	253.80	J/mol×K	524.82	Joback Method
cpg	264.99	J/mol×K	559.51	Joback Method
cpg	275.53	J/mol×K	594.21	Joback Method
cpg	285.44	J/mol×K	628.90	Joback Method
cpg	294.74	J/mol×K	663.60	Joback Method
cpg	303.46	J/mol×K	698.29	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=C1737195&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