2',5'-difluoropropiophenone

Inchi: InChI=1S/C9H8F2O/c1-2-9(12)7-5-6(10)3-4-8(7)11/h3-5H,2H2,1H3
InchiKey: BXLHXHGCQFJTLA-UHFFFAOYSA-N
Formula: C9H8F2O
SMILES: CCC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 170.16
CAS: 29112-90-1

Physical Properties

Property code	Value	Unit	Source
gf	-400.49	kJ/mol	Joback Method
hf	-520.30	kJ/mol	Joback Method
hfus	20.09	kJ/mol	Joback Method
hvap	44.34	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.558		Crippen Method
mcvol	119.020	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	494.37	K	Joback Method
tc	693.12	K	Joback Method
tf	293.76	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.27	J/mol×K	494.37	Joback Method
cpg	261.17	J/mol×K	527.50	Joback Method
cpg	271.50	J/mol×K	560.62	Joback Method
cpg	281.27	J/mol×K	593.75	Joback Method
cpg	290.51	J/mol×K	626.87	Joback Method
cpg	299.22	J/mol×K	660.00	Joback Method
cpg	307.42	J/mol×K	693.12	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=C29112901&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
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