3,5-Difluoro-4-hydroxypropiophenone

Inchi: InChI=1S/C9H8F2O2/c1-2-8(12)5-3-6(10)9(13)7(11)4-5/h3-4,13H,2H2,1H3
InchiKey: PJIDRPUAOWTRGM-UHFFFAOYSA-N
Formula: C9H8F2O2
SMILES: CCC(=O)c1cc(F)c(O)c(F)c1
Mol. weight [g/mol]: 186.16
CAS: 178374-78-2

Physical Properties

Property code	Value	Unit	Source
gf	-555.11	kJ/mol	Joback Method
hf	-697.61	kJ/mol	Joback Method
hfus	25.87	kJ/mol	Joback Method
hvap	57.35	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.263		Crippen Method
mcvol	124.890	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
tb	574.99	K	Joback Method
tc	785.81	K	Joback Method
tf	405.48	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.33	J/mol×K	574.99	Joback Method
cpg	306.11	J/mol×K	610.13	Joback Method
cpg	315.27	J/mol×K	645.26	Joback Method
cpg	323.85	J/mol×K	680.40	Joback Method
cpg	331.90	J/mol×K	715.54	Joback Method
cpg	339.50	J/mol×K	750.67	Joback Method
cpg	346.67	J/mol×K	785.81	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=C178374782&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