2'-Fluoro-2-hydroxy-4-methoxybenzophenone

Inchi: InChI=1S/C14H11FO3/c1-18-9-6-7-11(13(16)8-9)14(17)10-4-2-3-5-12(10)15/h2-8,16H,1
InchiKey: VVOYPINUWBAVQM-UHFFFAOYSA-N
Formula: C14H11FO3
SMILES: COc1ccc(C(=O)c2ccccc2F)c(O)c1
Mol. weight [g/mol]: 246.23
CAS: 3119-88-8

Physical Properties

Property code	Value	Unit	Source
gf	-310.79	kJ/mol	Joback Method
hf	-500.39	kJ/mol	Joback Method
hfus	30.97	kJ/mol	Joback Method
hvap	73.99	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.771		Crippen Method
mcvol	175.680	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	739.22	K	Joback Method
tc	979.74	K	Joback Method
tf	509.89	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.44	J/mol×K	939.65	Joback Method
cpg	469.26	J/mol×K	739.22	Joback Method
cpg	481.44	J/mol×K	779.31	Joback Method
cpg	492.76	J/mol×K	819.39	Joback Method
cpg	503.31	J/mol×K	859.48	Joback Method
cpg	513.17	J/mol×K	899.57	Joback Method
cpg	531.21	J/mol×K	979.74	Joback Method
hsubt	109.30	kJ/mol	312.50	NIST Webbook

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=C3119888&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
hsubt:	Enthalpy of sublimation at a given temperature
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