4'-Hydroxy-3'-methoxyacetophenone, pentafluoropropionate

Inchi: InChI=1S/C12H9F5O4/c1-6(18)7-3-4-8(9(5-7)20-2)21-10(19)11(13,14)12(15,16)17/h3-5H

InchiKey: VYFGIABQVRLBMT-UHFFFAOYSA-N

Formula: C12H9F5O4

SMILES: COc1cc(C(C)=O)ccc1OC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 312.19

Physical Properties

Property code	Value	Unit	Source
gf	-1292.90	kJ/mol	Joback Method
hf	-1565.07	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	57.54	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.001		Crippen Method
mcvol	179.910	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
tb	653.07	K	Joback Method
tc	844.40	K	Joback Method
tf	428.57	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.29	J/mol×K	653.07	Joback Method
cpg	493.49	J/mol×K	684.96	Joback Method
cpg	503.91	J/mol×K	716.85	Joback Method
cpg	513.59	J/mol×K	748.73	Joback Method
cpg	522.55	J/mol×K	780.62	Joback Method
cpg	530.82	J/mol×K	812.51	Joback Method
cpg	538.44	J/mol×K	844.40	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=U375933&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume