4'-Hydroxy-3'-methoxyacetophenone, heptafluorobutyrate

Inchi: InChI=1S/C13H9F7O4/c1-6(21)7-3-4-8(9(5-7)23-2)24-10(22)11(14,15)12(16,17)13(18,19

InchiKey: OZXPCJJAUGSZNL-UHFFFAOYSA-N

Formula: C13H9F7O4

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

Mol. weight [g/mol]: 362.20

Physical Properties

Property code	Value	Unit	Source
gf	-1671.26	kJ/mol	Joback Method
hf	-1986.68	kJ/mol	Joback Method
hfus	27.58	kJ/mol	Joback Method
hvap	56.84	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.636		Crippen Method
mcvol	197.540	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	1465.00		NIST Webbook
tb	671.26	K	Joback Method
tc	855.52	K	Joback Method
tf	443.44	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.66	J/mol×K	671.26	Joback Method
cpg	562.74	J/mol×K	701.97	Joback Method
cpg	573.00	J/mol×K	732.68	Joback Method
cpg	582.49	J/mol×K	763.39	Joback Method
cpg	591.25	J/mol×K	794.10	Joback Method
cpg	599.32	J/mol×K	824.81	Joback Method
cpg	606.75	J/mol×K	855.52	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=U375932&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume