4'-Hydroxy-3'-methoxyacetophenone, trifluoroacetate

Inchi: InChI=1S/C11H9F3O4/c1-6(15)7-3-4-8(9(5-7)17-2)18-10(16)11(12,13)14/h3-5H,1-2H3
InchiKey: SOSFUWVSIGJFHZ-UHFFFAOYSA-N
Formula: C11H9F3O4
SMILES: COc1cc(C(C)=O)ccc1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 262.18

Physical Properties

Property code	Value	Unit	Source
gf	-914.54	kJ/mol	Joback Method
hf	-1143.46	kJ/mol	Joback Method
hfus	24.91	kJ/mol	Joback Method
hvap	58.25	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.365		Crippen Method
mcvol	162.280	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
rinpol	1407.00		NIST Webbook
rinpol	1407.00		NIST Webbook
tb	634.88	K	Joback Method
tc	834.77	K	Joback Method
tf	413.70	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.66	J/mol×K	634.88	Joback Method
cpg	424.89	J/mol×K	668.20	Joback Method
cpg	435.40	J/mol×K	701.51	Joback Method
cpg	445.22	J/mol×K	734.83	Joback Method
cpg	454.35	J/mol×K	768.14	Joback Method
cpg	462.81	J/mol×K	801.46	Joback Method
cpg	470.61	J/mol×K	834.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375934&Units=SI
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

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