2',6'-Dihydroxyacetophenone, diacetate

Inchi: InChI=1S/C12H12O5/c1-7(13)12-10(16-8(2)14)5-4-6-11(12)17-9(3)15/h4-6H,1-3H3
InchiKey: BQSKGNHSFVZDGZ-UHFFFAOYSA-N
Formula: C12H12O5
SMILES: CC(=O)Oc1cccc(OC(C)=O)c1C(C)=O
Mol. weight [g/mol]: 236.22

Physical Properties

Property code	Value	Unit	Source
gf	-453.45	kJ/mol	Joback Method
hf	-679.60	kJ/mol	Joback Method
hfus	27.27	kJ/mol	Joback Method
hvap	70.96	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	1.740		Crippen Method
mcvol	172.630	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1635.50		NIST Webbook
tb	717.05	K	Joback Method
tc	935.93	K	Joback Method
tf	470.71	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.81	J/mol×K	717.05	Joback Method
cpg	499.29	J/mol×K	899.45	Joback Method
cpg	490.90	J/mol×K	862.97	Joback Method
cpg	481.65	J/mol×K	826.49	Joback Method
cpg	471.55	J/mol×K	790.01	Joback Method
cpg	460.60	J/mol×K	753.53	Joback Method
cpg	506.81	J/mol×K	935.93	Joback Method
dvisc	0.0001502	Pa×s	717.05	Joback Method
dvisc	0.0001834	Pa×s	675.99	Joback Method

dvisc	0.0002297	Pa×s	634.94	Joback Method
dvisc	0.0002968	Pa×s	593.88	Joback Method
dvisc	0.0003984	Pa×s	552.82	Joback Method
dvisc	0.0005606	Pa×s	511.77	Joback Method
dvisc	0.0008374	Pa×s	470.71	Joback Method

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=U352811&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
dvisc:	Dynamic viscosity
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