2',4'-Dihydroxyacetophenone, diacetate

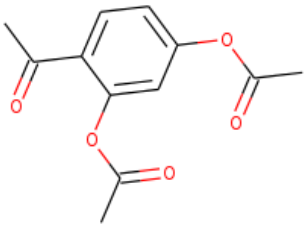
InChI: InChI=1S/C12H12O5/c1-7(13)11-5-4-10(16-8(2)14)6-12(11)17-9(3)15/h4-6H,1-3H3

InChI Key: FKSHOQTWUWCWTG-UHFFFAOYSA-N

Formula: C12H12O5

SMILES: CC(=O)Oc1ccc(C(C)=O)c(OC(C)=O)c1

Molecular Weight: 236.22



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-453.45	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-679.60	kJ/mol	Joback Method
$\Delta_{fus} H°$	27.27	kJ/mol	Joback Method
$\Delta_{vap} H°$	70.96	kJ/mol	Joback Method
$logP_{oct/wat}$	1.74		Crippen Method
P_c	2729.71	kPa	Joback Method
T_{boil}	717.05	K	Joback Method
T_c	935.93	K	Joback Method
T_{fus}	470.71	K	Joback Method
V_c	0.65	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	448.81	J/mol×K	717.05	Joback Method
η	0.00	Pa×s	717.05	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H12O5/c1-7(13)11-5-4-10(16-8(2)14)6-12(11)17-9(3)15/h4-6H,1-3H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).