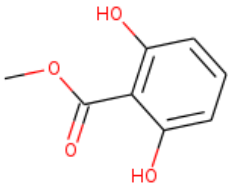
Benzoic acid, 2,6-dihydroxy-, methyl ester

Other names: 2,6-Dihydroxybenzoic acid methyl ester; Methyl 2,6-dihydroxybenzoate; «gamma»-Resorcylic acid, methyl ester.
InChI: InChI=1S/C8H8O4/c1-12-8(11)7-5(9)3-2-4-6(7)10/h2-4,9-10H,1H3
InChI Key: WCQZCKUNZVMBDC-UHFFFAOYSA-N
Formula: C8H8O4
SMILES: COC(=O)c1c(O)cccc1O
Molecular Weight: 168.15
CAS: 2150-45-0



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-414.27	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-571.34	kJ/mol	Joback Method
$\Delta_{fus} H°$	24.87	kJ/mol	Joback Method
$\Delta_{vap} H°$	70.86	kJ/mol	Joback Method
$logP_{oct/wat}$	0.88		Crippen Method
P_c	5818.28	kPa	Joback Method
T_{boil}	646.65	K	Joback Method
T_c	888.33	K	Joback Method
T_{fus}	501.94	K	Joback Method
V_c	0.33	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	299.69	J/mol×K	646.65	Joback Method
η	0.00	Pa×s	646.65	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H8O4/c1-12-8(11)7-5(9)3-2-4-6(7)10/h2-4,9-10H,1H3
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).