

Benzoic acid, 2-hydroxy-, 1-methylethyl ester

Other names: Isopropyl o-hydroxybenzoate; Isopropyl salicylate; Salicylic acid, isopropyl ester.

InChI:

InChI=1S/C10H12O3/c1-7(2)13-10(12)8-5-3-4-6-9(8)11/h3-7,11H,1-2H3

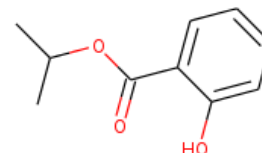
InChI Key: YEULQIJMIOWCHB-UHFFFAOYSA-N

Formula: C10H12O3

SMILES: CC(C)OC(=O)c1ccccc1O

Molecular Weight: 180.20

CAS: 607-85-2



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-245.25	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-440.59	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	20.74	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	61.91	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.96		Crippen Method
P_c	3699.95	kPa	Joback Method
T_{boil}	611.35	K	Joback Method
T_c	839.56	K	Joback Method
T_{fus}	397.76	K	Joback Method
V_c	0.47	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	350.96	J/mol×K	611.35	Joback Method
η	0.00	Paxs	611.35	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H12O3/c1-7\(2\)13-10\(12\)8-5-3-4-6-9\(8\)11/h3-7,11H,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H12O3/c1-7(2)13-10(12)8-5-3-4-6-9(8)11/h3-7,11H,1-2H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

$C_{p, gas}$: Ideal gas heat capacity (J/molxK).

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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