Benzoic acid, 2-hydroxy-, ethyl ester

Other names: 2-Hydroxybenzoic acid ethyl ester; Ethyl 2-hydroxybenzoate; Ethyl o-hydroxybenzoate; Ethyl salicylate; Mesotol; NSC 8209; Sal ethyl; Salicylic acid, ethyl ester; Salicylic ether; Salotan; o-(Ethoxycarbonyl)phenol.

InChI: InChI=1S/C9H10O3/c1-2-12-9(11)7-5-3-4-6-8(7)10/h3-6,10H,2H2,1H3

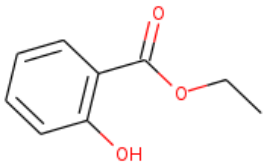
InChI Key: GYCKQBWUSACYIF-UHFFFAOYSA-N

Formula: C9H10O3

SMILES: CCOC(=O)c1ccccc1O

Molecular Weight: 166.17

CAS: 118-61-6



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-251.23	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-414.67	kJ/mol	Joback Method
$\Delta_{fus} H°$	21.68	kJ/mol	Joback Method
$\Delta_{vap} H°$	60.07	kJ/mol	Joback Method
$logP_{oct/wat}$	1.57		Crippen Method
P_c	4130.29	kPa	Joback Method
T_{boil}	507.20	K	NIST Webbook
T_{boil}	506.95 ± 0.50	K	NIST Webbook
T_{boil}	495.50 ± 0.50	K	NIST Webbook
T_{boil}	506.90 ± 1.00	K	NIST Webbook
T_{boil}	504.65 ± 1.50	K	NIST Webbook
T_c	816.64	K	Joback Method
T_{fus}	401.49	K	Joback Method
V_c	0.42	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	304.03	J/mol×K	588.91	Joback Method
η	0.00	Pa×s	588.91	Joback Method
$\Delta_{vap}H$	59.20	kJ/mol	310.5	NIST Webbook
$\Delta_{vap}H$	55.20	kJ/mol	419.5	NIST Webbook
$\Delta_{vap}H$	53.40	kJ/mol	446.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H10O3/c1-2-12-9(11)7-5-3-4-6-8(7)10/h3-6,10H,2H2,1H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°$_{gas}$**: Enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (kJ/mol).
Δ_{vap}**H**: Enthalpy of vaporization at a given temperature (kJ/mol).
***log*P$_{oct/wat}$**: 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 (m^3/kg-mol).

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