Benzoic acid, 2-hydroxy-, ethyl ester

Other names:	2-Hydroxybenzoic acid ethyl ester
	Ethyl o-hydroxybenzoate
	NSC 8209
	ethyl 2-hydroxybenzoate
	ethyl salicylate
	mesotol
	o-(ethoxycarbonyl)phenol
	sal ethyl
	salicylic acid, ethyl ester
	salicylic ether
	salotan
Inchi:	InChI=1S/C9H10O3/c1-2-12-9(11)7-5-3-4-6-8(7)10/h3-6,10H,2H2,1H3
InchiKey:	GYCKQBWUSACYIF-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	CCOC(=O)c1ccccc1O
Mol. weight [g/mol]:	166.17
CAS:	118-61-6

Physical Properties

Property code	Value	Unit	Source
gf	-251.23	kJ/mol	Joback Method
hf	-414.67	kJ/mol	Joback Method
hfus	21.68	kJ/mol	Joback Method
hvap	60.07	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.569		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	1286.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1236.80		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1270.00		NIST Webbook

rinpol	1279.00	NIST Webbook
rinpol	1269.00	NIST Webbook
rinpol	1272.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1265.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1238.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1280.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1279.00	NIST Webbook
rinpol	1255.00	NIST Webbook
rinpol	1286.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1286.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1272.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1254.00	NIST Webbook
rinpol	1280.00	NIST Webbook
rinpol	1272.00	NIST Webbook
rinpol	1249.10	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1265.00	NIST Webbook
rinpol	1269.00	NIST Webbook
ripol	1828.00	NIST Webbook
ripol	1832.00	NIST Webbook
ripol	1837.00	NIST Webbook
ripol	1791.00	NIST Webbook
ripol	1786.00	NIST Webbook
ripol	1786.00	NIST Webbook
ripol	1820.00	NIST Webbook
ripol	1778.00	NIST Webbook
ripol	1834.00	NIST Webbook
ripol	1780.00	NIST Webbook
ripol	1787.00	NIST Webbook
ripol	1834.00	NIST Webbook
ripol	1834.00	NIST Webbook

ripol	1834.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1832.00		NIST Webbook
ripol	1829.00		NIST Webbook
ripol	1828.00		NIST Webbook
ripol	1798.00		NIST Webbook
ripol	1798.00		NIST Webbook
ripol	1788.00		NIST Webbook
ripol	1816.00		NIST Webbook
ripol	1828.00		NIST Webbook
ripol	1815.00		NIST Webbook
tb	504.65 ± 1.50	K	NIST Webbook
tb	506.95 ± 0.50	K	NIST Webbook
tb	495.50 ± 0.50	K	NIST Webbook
tb	506.90 ± 1.00	K	NIST Webbook
tb	507.20	K	NIST Webbook
tc	816.64	K	Joback Method
tf	401.49	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.35	J/mol×K	816.64	Joback Method
cpg	325.77	J/mol×K	664.82	Joback Method
cpg	315.28	J/mol×K	626.86	Joback Method
cpg	304.03	J/mol×K	588.91	Joback Method
cpg	353.29	J/mol×K	778.68	Joback Method
cpg	344.71	J/mol×K	740.73	Joback Method
cpg	335.56	J/mol×K	702.77	Joback Method
dvisc	0.0028310	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K

dvisc	0.0022530	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K	
dvisc	0.0018420	Pa×s	318.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K	
dvisc	0.0036940	Pa×s	288.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K	
hvapt	65.30	kJ/mol	310.00	Gas-phase enthalpies of formation of ethyl hydroxybenzoates: An experimental and theoretical approach	
hvapt	59.20	kJ/mol	310.50	NIST Webbook	
hvapt	55.20	kJ/mol	419.50	NIST Webbook	
hvapt	53.40	kJ/mol	446.00	NIST Webbook	

rhol	1125.00	kg/m3	298.15	Refractive Indices and Surface Tensions of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K	
srf	0.04	N/m	308.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K	
srf	0.04	N/m	288.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K	
srf	0.03	N/m	358.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K	
srf	0.03	N/m	348.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K	
srf	0.03	N/m	338.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K	

srf	0.03	N/m	328.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.04	N/m	298.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	318.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K

Sources

Gas-phase enthalpies of formation of ethyl hydroxybenzoates: An experimental and theoretical approach:	https://www.doi.org/10.1016/j.jct.2017.09.007
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C118616&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Refractive Indices and Surface Tensions of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je060139a
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je050402s
Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K:	https://www.doi.org/10.1021/je050170x

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume