Ethylparaben

Other names:	4-(Ethoxycarbonyl)phenol
	4-Carbethoxyphenol
	4-Hydroxybenzoic acid, ethyl ester
	Aseptin A
	Aseptine A
	Aseptoform E
	Benzoic acid, 4-hydroxy-, ethyl ester
	Benzoic acid, p-hydroxy-, ethyl ester
	Bonomold OE
	Easeptol
	Ester etylowykwasu p-hydroksybenzoesowego
	Ethyl 4-hydroxybenzoate
	Ethyl Butex
	Ethyl p-hydroxybenzoate
	Ethyl p-oxybenzoate
	Ethyl para-hydroxybenzoate
	Ethyl parasept
	Ethyl-p-hydroxybenzoate
	Ethylester kyseliny p-hydroxybenzoove
	Mekkings E
	Mycocten
	NSC 23514
	Napagin A
	Nipagin A
	Nipagina A
	Nipazin A
	Para-hydroxybenzoic acid ethyl ester
	Sobrol A
	Solbrol A
	Tegosept E
	p-Carbethoxyphenol
	p-Hydroxybenzoate ethyl ester
	p-Hydroxybenzoic acid ethyl ester
	p-Oxybenzoesaeureaethylester
Inchi:	InChI=1S/C9H10O3/c1-2-12-9(11)7-3-5-8(10)6-4-7/h3-6,10H,2H2,1H3
InchiKey:	NUVBSKCKDOMJSU-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	CCOC(=O)c1ccc(O)cc1
Mol. weight [g/mol]:	166.17
CAS:	120-47-8

Physical Properties

Property code	Value	Unit	Source
gf	-251.23	kJ/mol	Joback Method
hf	-414.67	kJ/mol	Joback Method
hfus	100.90 ± 0.70	kJ/mol	NIST Webbook
hvap	60.07	kJ/mol	Joback Method
log10ws	-2.35		Estimated Solubility Method
log10ws	-2.35		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.10		Aqueous Solubility Prediction Method
logp	1.569		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	1467.00		NIST Webbook
rinpol	1467.00		NIST Webbook
tb	570.70	K	NIST Webbook
tc	816.64	K	Joback Method
tf	388.65	K	Ternary phase diagrams of ethyl paraben and propyl paraben in ethanol aqueous solvents
tf	388.80	K	Solubility and preferential solvation of some n-alkyl-parabens in methanol + water mixtures at 298.15 K
tf	389.95	K	Aqueous Solubility Prediction Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.56	J/mol×K	702.77	Joback Method
cpg	361.35	J/mol×K	816.64	Joback Method
cpg	353.29	J/mol×K	778.68	Joback Method
cpg	344.71	J/mol×K	740.73	Joback Method

cpg	304.03	J/mol×K	588.91	Joback Method
cpg	315.28	J/mol×K	626.86	Joback Method
cpg	325.77	J/mol×K	664.82	Joback Method
dvisc	0.0000400	Pa×s	588.91	Joback Method
dvisc	0.0001481	Pa×s	495.20	Joback Method
dvisc	0.0000909	Pa×s	526.44	Joback Method
dvisc	0.0000590	Pa×s	557.67	Joback Method
dvisc	0.0010100	Pa×s	401.49	Joback Method
dvisc	0.0004856	Pa×s	432.73	Joback Method
dvisc	0.0002577	Pa×s	463.96	Joback Method
hfust	26.40	kJ/mol	389.00	NIST Webbook
hfust	27.90	kJ/mol	389.20	NIST Webbook
hfust	32.49	kJ/mol	388.90	NIST Webbook
hvapt	72.70	kJ/mol	400.00	Gas-phase enthalpies of formation of ethyl hydroxybenzoates: An experimental and theoretical approach

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Parabens in Subcritical Water:	https://www.doi.org/10.1021/je4010883
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubility and preferential solvation of some n-alkyl-parabens in methanol + water mixtures at 298.15 K:	https://www.doi.org/10.1016/j.jct.2017.01.005
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Gas-phase enthalpies of formation of ethyl hydroxybenzoates: An experimental and theoretical approach:	https://www.doi.org/10.1016/j.jct.2017.09.007
Single component and mixture solubilities of ethyl p-hydroxybenzoate and ethyl p-aminobenzoate in supercritical CO2:	https://www.doi.org/10.1016/j.fluid.2007.09.020
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120478&Units=SI
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
Ternary phase diagrams of ethyl paraben and propyl paraben in ethanol aqueous solvents:	https://www.doi.org/10.1016/j.fluid.2014.05.036

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
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume