methyl 4-hydroxybenzoate

Other names:	Benzoic acid, 4-hydroxy-, methyl ester
	Methylparaben
	methyl p-hydroxybenzoate
	p-hydroxybenzoic acid methyl ester
Inchi:	InChI=1S/C8H8O3/c1-11-8(10)6-2-4-7(9)5-3-6/h2-5,9H,1H3
InchiKey:	LXCFILQKKLGQFO-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	COC(=O)c1ccc(O)cc1
Mol. weight [g/mol]:	152.15
CAS:	99-76-3

Physical Properties

Property code	Value	Unit	Source
affp	863.40	kJ/mol	NIST Webbook
basg	832.50	kJ/mol	NIST Webbook
gf	-259.65	kJ/mol	Joback Method
hf	-394.03	kJ/mol	Joback Method
hfus	26.40	kJ/mol	Thermodynamic properties of the methyl esters of p-hydroxy and p-methoxy benzoic acids
hsub	98.80 ± 0.80	kJ/mol	NIST Webbook
hvap	83.10	kJ/mol	NIST Webbook
log10ws	-1.83		Estimated Solubility Method
log10ws	-1.78		Aqueous Solubility Prediction Method
logp	1.179		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
rinpol	1460.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1410.00		NIST Webbook

rinpol	1470.40		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1435.00		NIST Webbook
ripol	2911.00		NIST Webbook
ripol	2932.00		NIST Webbook
ripol	2932.00		NIST Webbook
ripol	2911.00		NIST Webbook
ripol	2925.00		NIST Webbook
ripol	2930.00		NIST Webbook
tb	566.03	K	Joback Method
tc	798.25	K	Joback Method
tf	402.77	K	Aqueous Solubility Prediction Method
tf	398.90	K	Solubility and preferential solvation of some n-alkyl-parabens in methanol + water mixtures at 298.15 K
tf	399.00	K	Experimental and theoretical study of methyl n-hydroxybenzoates
tf	398.40 ± 0.50	K	NIST Webbook
tf	398.60	K	The standard molar enthalpy of the base catalysed hydrolysis of methyl paraben revisited
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.95	J/mol×K	759.54	Joback Method
cpg	259.25	J/mol×K	566.03	Joback Method
cpg	269.54	J/mol×K	604.73	Joback Method
cpg	279.09	J/mol×K	643.44	Joback Method
cpg	287.96	J/mol×K	682.14	Joback Method
cpg	296.23	J/mol×K	720.84	Joback Method
cpg	311.19	J/mol×K	798.25	Joback Method

cps	214.41	J/mol×K	298.15	Evaluation of sublimation enthalpy by thermogravimetry: Analysis of the diffusion effects in the case of methyl and phenyl substituted hydantoins
dvisc	0.0000501	Pa×s	566.03	Joback Method
dvisc	0.0011881	Pa×s	390.22	Joback Method
dvisc	0.0005829	Pa×s	419.52	Joback Method
dvisc	0.0003139	Pa×s	448.82	Joback Method
dvisc	0.0001823	Pa×s	478.12	Joback Method
dvisc	0.0001128	Pa×s	507.43	Joback Method
dvisc	0.0000735	Pa×s	536.73	Joback Method
hfust	24.31	kJ/mol	398.50	NIST Webbook
hfust	25.30	kJ/mol	399.20	NIST Webbook
hfust	24.31	kJ/mol	398.50	NIST Webbook
hvapt	81.50	kJ/mol	481.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Evaluation of sublimation enthalpy by thermogravimetry: Analysis of the diffusion effects in the case of methyl and phenyl substituted hydantoins:	https://www.doi.org/10.1016/j.tca.2017.06.024
Solubility of the Drugs Bisacodyl, Methimazole, Methylparaben and Propylparaben in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je020080h
Solubility of Parabens in Supercritical Water:	https://www.doi.org/10.1021/je4010883
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Thermodynamic properties of the methyl esters of p-hydroxy and p-methoxy benzoic acids:	https://www.doi.org/10.1016/j.jct.2014.06.002
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99763&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
The standard molar enthalpy of the base catalysed hydrolysis of methyl paraben revisited:	https://www.doi.org/10.1016/j.jct.2016.07.042
Experimental and theoretical study of methyl n-hydroxybenzoates:	https://www.doi.org/10.1016/j.jct.2018.04.011

Legend

affp:	Proton affinity

basg:	Gas basicity
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hsub:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume