Benzoic acid, 3-hydroxy-, methyl ester

Other names:	3-(Methoxycarbonyl)phenol
	3-HO-C6H4-COOCH3
	3-hydroxybenzoic acid methyl ester
	Benzoic acid, m-hydroxy-, methyl ester
	Methyl m-oxybenzoate
	NSC 40536
	m-Carbomethoxyphenol
	m-hydroxybenzoic acid methyl ester
	methyl 3-hydroxybenzoate
	methyl m-hydroxybenzoate
Inchi:	InChI=1S/C8H8O3/c1-11-8(10)6-3-2-4-7(9)5-6/h2-5,9H,1H3
InchiKey:	YKUCHDXIBAQWSF-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	COC(=O)c1cccc(O)c1
Mol. weight [g/mol]:	152.15
CAS:	19438-10-9

Physical Properties

Property code	Value	Unit	Source
affp	850.00	kJ/mol	NIST Webbook
basg	819.10	kJ/mol	NIST Webbook
gf	-259.65	kJ/mol	Joback Method
hf	-394.03	kJ/mol	Joback Method
hfus	19.09	kJ/mol	Joback Method
hvap	57.85	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.179		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
rinpol	1389.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1384.00		NIST Webbook
ripol	2012.00		NIST Webbook

tb	566.03	K	Joback Method
tc	798.25	K	Joback Method
tf	344.25	K	Experimental and theoretical study of methyl n-hydroxybenzoates
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	303.95	J/mol×K	759.54	Joback Method
cpg	311.19	J/mol×K	798.25	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
dvisc	0.0000501	Pa×s	566.03	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	553.20	K	94.50	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Experimental and theoretical study of methyl n-hydroxybenzoates: https://www.doi.org/10.1016/j.jct.2018.04.011

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19438109&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume