

meth yl salicylate

Other names:	2-Hydroxybenzoic acid methyl ester 2-carbomethoxyphenol Benzoic acid, 2-hydroxy-, methyl ester methyl 2-hydroxybenzoate methyl o-hydroxybenzoate methyl ortho-hydroxybenzoate salicylic acid methyl ester
Inchi:	InChI=1S/C8H8O3/c1-11-8(10)6-4-2-3-5-7(6)9/h2-5,9H,1H3
InchiKey:	OSWPMRLSEDHDFH-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	COC(=O)c1ccccc1O
Mol. weight [g/mol]:	152.15
CAS:	119-36-8

Physical Properties

Property code	Value	Unit	Source
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
ie	7.65	eV	NIST Webbook
log10ws	-2.34		Aqueous Solubility Prediction Method
logp	1.179		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
rinpol	1163.10		NIST Webbook
rinpol	1169.35		NIST Webbook
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tb	496.50	K	NIST Webbook
tb	496.10 ± 0.50	K	NIST Webbook
tb	495.50 ± 0.50	K	NIST Webbook
tb	495.20	K	NIST Webbook
tc	709.00 ± 5.00	K	NIST Webbook
tf	271.49	K	Experimental and theoretical study of methyl n-hydroxybenzoates
tf	264.90	K	Aqueous Solubility Prediction Method
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	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
cpg	269.54	J/mol×K	604.73	Joback Method
cpl	248.90	J/mol×K	295.20	NIST Webbook
cpl	268.60	J/mol×K	295.20	NIST Webbook
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
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dvisc	0.0000735	Pa×s	536.73	Joback Method
dvisc	0.0000501	Pa×s	566.03	Joback Method
hvapt	59.90	kJ/mol	412.00	NIST Webbook
hvapt	58.70	kJ/mol	412.50	NIST Webbook
hvapt	56.90	kJ/mol	310.50	NIST Webbook
rhoI	1169.37	kg/m3	308.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model

rhoI	1154.42	kg/m3	323.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1159.40	kg/m3	318.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	4.51315e+02
Coeff. B	-2.72868e+04
Coeff. C	-6.47318e+01
Coeff. D	4.09395e-05
Temperature range (K), min.	265.15
Temperature range (K), max.	701.00

Sources

Experimental and theoretical study of methyl n-hydroxybenzoates:	https://www.doi.org/10.1016/j.jct.2018.04.011
Green Leaf Volatiles on Atmospheric Air/Water Interfaces: A Combined KDB Vapor Pressure and Polar Simulation Study:	https://www.doi.org/10.1021/je500114m
Solubility of Methyl Salicylate in Supercritical Carbon Dioxide at Several Temperatures:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1141
Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model:	https://www.doi.org/10.1021/je800476n
Crippen Method:	https://www.doi.org/10.1021/je4003256
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solute-Solvent and Solvent-Solvent Interactions of Menthol in Isopropyl KDB and its Binary Mixtures with Methyl Salicylate by Volumetric, Viscometric, Interferometric and Refractive Index Techniques.:	http://link.springer.com/article/10.1007/BF02311772
	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
	https://www.doi.org/10.1016/j.tca.2009.12.001
	https://www.cheric.org/files/research/kdb/mol/mol1141.mol
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119368&Units=SI

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid 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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
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

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