Benzoic acid, 2,4-dihydroxy-, methyl ester

Other names:	«beta»-Resorcylic acid, methyl ester
	Methyl «beta»-resorcylate
	Methyl 2,4-dihydroxybenzoate
	2,4-Dihydroxybenzoic acid methyl ester
	Methyl benzoate, 2,4-dihydroxy-
Inchi:	InChI=1S/C8H8O4/c1-12-8(11)6-3-2-5(9)4-7(6)10/h2-4,9-10H,1H3
InchiKey:	IIFCLXHRIYTHPV-UHFFFAOYSA-N
Formula:	C8H8O4
SMILES:	COC(=O)c1ccc(O)cc1O
Mol. weight [g/mol]:	168.15
CAS:	2150-47-2

Physical Properties

Property code	Value	Unit	Source
gf	-414.27	kJ/mol	Joback Method
hf	-571.34	kJ/mol	Joback Method
hfus	24.87	kJ/mol	Joback Method
hvap	70.86	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	0.884		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	5818.28	kPa	Joback Method
ripol	2898.00		NIST Webbook
tb	646.65	K	Joback Method
tc	888.33	K	Joback Method
tf	501.94	K	Joback Method
vc	0.332	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.69	J/mol×K	646.65	Joback Method
cpg	308.47	J/mol×K	686.93	Joback Method
cpg	316.66	J/mol×K	727.21	Joback Method

cpg	324.37	J/mol×K	767.49	Joback Method
cpg	331.74	J/mol×K	807.77	Joback Method
cpg	338.88	J/mol×K	848.05	Joback Method
cpg	345.91	J/mol×K	888.33	Joback Method
dvisc	0.0000678	Pa×s	501.94	Joback Method
dvisc	0.0000375	Pa×s	526.06	Joback Method
dvisc	0.0000218	Pa×s	550.18	Joback Method
dvisc	0.0000133	Pa×s	574.29	Joback Method
dvisc	0.0000084	Pa×s	598.41	Joback Method
dvisc	0.0000055	Pa×s	622.53	Joback Method
dvisc	0.0000038	Pa×s	646.65	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C2150472&Units=SI

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume