Benzoic acid, 2,3-dihydroxy-, methyl ester

Other names:	o-Pyrocatechuic acid, methyl ester
	Methyl 2,3-dihydroxybenzoate
Inchi:	InChI=1S/C8H8O4/c1-12-8(11)5-3-2-4-6(9)7(5)10/h2-4,9-10H,1H3
InchiKey:	DOAJWTSNTNAEIY-UHFFFAOYSA-N
Formula:	C8H8O4
SMILES:	COC(=O)c1cccc(O)c1O
Mol. weight [g/mol]:	168.15
CAS:	2411-83-8

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
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	338.88	J/mol×K	848.05	Joback Method
cpg	331.74	J/mol×K	807.77	Joback Method
cpg	324.37	J/mol×K	767.49	Joback Method
cpg	316.66	J/mol×K	727.21	Joback Method
cpg	308.47	J/mol×K	686.93	Joback Method
cpg	345.91	J/mol×K	888.33	Joback Method

dvisc	0.0000038	Pa×s	646.65	Joback Method
dvisc	0.0000055	Pa×s	622.53	Joback Method
dvisc	0.0000084	Pa×s	598.41	Joback Method
dvisc	0.0000133	Pa×s	574.29	Joback Method
dvisc	0.0000218	Pa×s	550.18	Joback Method
dvisc	0.0000375	Pa×s	526.06	Joback Method
dvisc	0.0000678	Pa×s	501.94	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=C2411838&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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