Benzoic acid, 4-hydroxy-3,5-dimethoxy-, methyl ester

Other names: Methyl syringate
Methyl 4-hydroxy-3,5-dimethoxybenzoate
Syringic acid monomethyl ester
Methyl 3,5-dimethoxy-4-hydroxybenzoate
Methyl syringoate

Inchi: InChI=1S/C10H12O5/c1-13-7-4-6(10(12)15-3)5-8(14-2)9(7)11/h4-5,11H,1-3H3

InchiKey: ZMXJAEGJWHJMGX-UHFFFAOYSA-N

Formula: C10H12O5

SMILES: COC(=O)c1cc(OC)c(O)c(OC)c1

Mol. weight [g/mol]: 212.20

CAS: 884-35-5

Physical Properties

Property code	Value	Unit	Source
gf	-472.07	kJ/mol	Joback Method
hf	-722.69	kJ/mol	Joback Method
hfus	25.87	kJ/mol	Joback Method
hvap	68.44	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.196		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	1725.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
ripol	2957.00		NIST Webbook
ripol	2933.00		NIST Webbook
ripol	2957.00		NIST Webbook
ripol	2933.00		NIST Webbook
ripol	2957.00		NIST Webbook
tb	666.59	K	Joback Method
tc	886.20	K	Joback Method
tf	482.26	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.06	J/mol×K	666.59	Joback Method
cpg	446.23	J/mol×K	849.60	Joback Method
cpg	437.18	J/mol×K	813.00	Joback Method
cpg	427.55	J/mol×K	776.40	Joback Method
cpg	417.33	J/mol×K	739.79	Joback Method
cpg	406.51	J/mol×K	703.19	Joback Method
cpg	454.70	J/mol×K	886.20	Joback Method
dvisc	0.0000149	Pa×s	666.59	Joback Method
dvisc	0.0000203	Pa×s	635.87	Joback Method
dvisc	0.0000287	Pa×s	605.15	Joback Method
dvisc	0.0000419	Pa×s	574.42	Joback Method
dvisc	0.0000641	Pa×s	543.70	Joback Method
dvisc	0.0001030	Pa×s	512.98	Joback Method
dvisc	0.0001758	Pa×s	482.26	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C884355&Units=SI
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

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
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