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

Other names:	Methyl 2,4-dimethoxybenzoate
	2,4-Dimethoxybenzoic acid methyl ester
	2,4-Dihydroxybenzoic acid, dimethyl ether, methyl ester
Inchi:	InChI=1S/C10H12O4/c1-12-7-4-5-8(10(11)14-3)9(6-7)13-2/h4-6H,1-3H3
InchiKey:	IHIJFZWLGPEYPJ-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	COC(=O)c1ccc(OC)cc1OC
Mol. weight [g/mol]:	196.20
CAS:	2150-41-6

Physical Properties

Property code	Value	Unit	Source
gf	-317.45	kJ/mol	Joback Method
hf	-545.38	kJ/mol	Joback Method
hfus	20.08	kJ/mol	Joback Method
hvap	55.43	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.490		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	1621.00		NIST Webbook
rinpol	1614.50		NIST Webbook
rinpol	1621.00		NIST Webbook
tb	585.97	K	Joback Method
tc	796.18	K	Joback Method
tf	370.54	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.19	J/mol×K	585.97	Joback Method
cpg	359.83	J/mol×K	621.00	Joback Method
cpg	371.90	J/mol×K	656.04	Joback Method

cpg	383.37	J/mol×K	691.07	Joback Method
cpg	394.23	J/mol×K	726.11	Joback Method
cpg	404.44	J/mol×K	761.14	Joback Method
cpg	413.99	J/mol×K	796.18	Joback Method
dvisc	0.0008149	Pa×s	370.54	Joback Method
dvisc	0.0005311	Pa×s	406.45	Joback Method
dvisc	0.0003711	Pa×s	442.35	Joback Method
dvisc	0.0002736	Pa×s	478.25	Joback Method
dvisc	0.0002105	Pa×s	514.16	Joback Method
dvisc	0.0001676	Pa×s	550.07	Joback Method
dvisc	0.0001372	Pa×s	585.97	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=C2150416&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

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume