Benzoic acid, 3,4,5-trimethoxy-, methyl ester

Other names:	3,4,5-Trimethoxybenzoic acid, methyl ester
	Methyl 3,4,5-trimethoxybenzoate
	Methyl tri-O-methylgallate
	Trimethylgallic acid methyl ester
Inchi:	InChI=1S/C11H14O5/c1-13-8-5-7(11(12)16-4)6-9(14-2)10(8)15-3/h5-6H,1-4H3
InchiKey:	KACHFMOHOPLTNX-UHFFFAOYSA-N
Formula:	C11H14O5
SMILES:	COC(=O)c1cc(OC)c(OC)c(OC)c1
Mol. weight [g/mol]:	226.23
CAS:	1916-07-0

Physical Properties

Property code	Value	Unit	Source
gf	-423.66	kJ/mol	Joback Method
hf	-709.71	kJ/mol	Joback Method
hfus	23.47	kJ/mol	Joback Method
hvap	60.73	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.499		Crippen Method
mcvol	167.140	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1669.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1678.00		NIST Webbook
tb	547.70	K	NIST Webbook
tc	841.99	K	Joback Method
tf	416.56	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.02	J/mol×K	636.25	Joback Method
cpg	432.20	J/mol×K	670.54	Joback Method

cpg	444.77	J/mol×K	704.83	Joback Method
cpg	456.70	J/mol×K	739.12	Joback Method
cpg	467.94	J/mol×K	773.41	Joback Method
cpg	478.45	J/mol×K	807.70	Joback Method
cpg	488.20	J/mol×K	841.99	Joback Method
dvisc	0.0005003	Pa×s	416.56	Joback Method
dvisc	0.0003420	Pa×s	453.18	Joback Method
dvisc	0.0002475	Pa×s	489.79	Joback Method
dvisc	0.0001874	Pa×s	526.40	Joback Method
dvisc	0.0001471	Pa×s	563.02	Joback Method
dvisc	0.0001189	Pa×s	599.63	Joback Method
dvisc	0.0000985	Pa×s	636.25	Joback Method

Sources

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=C1916070&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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