Benzenepropanoic acid, 3,4-dimethoxy-, methyl ester

Other names: Hydrocinnamic acid, 3,4-dimethoxy-, methyl ester
Methyl 3-(3,4-dimethoxyphenyl)propanoate
Propanoic acid, 3-(3,4-dimethoxyphenyl), methyl ester

Inchi: InChI=1S/C12H16O4/c1-14-10-6-4-9(8-11(10)15-2)5-7-12(13)16-3/h4,6,8H,5,7H2,1-3H3

InchiKey: VSWFXSSYWWNFNF-UHFFFAOYSA-N

Formula: C12H16O4

SMILES: COC(=O)CCc1ccc(OC)c(OC)c1

Mol. weight [g/mol]: 224.25

CAS: 27798-73-8

Physical Properties

Property code	Value	Unit	Source
gf	-300.61	kJ/mol	Joback Method
hf	-586.66	kJ/mol	Joback Method
hfus	25.26	kJ/mol	Joback Method
hvap	59.88	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	1.809		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1684.00		NIST Webbook
rinpol	1676.00		NIST Webbook
tb	631.73	K	Joback Method
tc	835.57	K	Joback Method
tf	393.08	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.38	J/mol×K	631.73	Joback Method
cpg	508.24	J/mol×K	801.60	Joback Method
cpg	496.95	J/mol×K	767.63	Joback Method

cpg	484.90	J/mol×K	733.65	Joback Method
cpg	472.11	J/mol×K	699.68	Joback Method
cpg	458.60	J/mol×K	665.70	Joback Method
cpg	518.77	J/mol×K	835.57	Joback Method
dvisc	0.0001137	Pa×s	631.73	Joback Method
dvisc	0.0001404	Pa×s	591.96	Joback Method
dvisc	0.0001787	Pa×s	552.18	Joback Method
dvisc	0.0002362	Pa×s	512.40	Joback Method
dvisc	0.0003272	Pa×s	472.63	Joback Method
dvisc	0.0004811	Pa×s	432.86	Joback Method
dvisc	0.0007650	Pa×s	393.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27798738&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume