2-Propenoic acid, 3-(4-hydroxyphenyl)-, methyl ester

Other names: 4-Hydroxycinnamic acid methyl ester
Cinnamic acid, p-hydroxy-, methyl ester
Methyl (2E)-3-(4-hydroxyphenyl)-2-propenoate
Methyl 4-coumarate
Methyl 4-hydroxycinnamate
Methyl ester of p-hydroxycinnamic acid
Methyl p-coumarate
Methyl p-hydroxycinnamate
NSC 154578
p-Coumaric acid methyl ester
p-Hydroxycinnamic acid methyl ester

Inchi: InChI=1S/C10H10O3/c1-13-10(12)7-4-8-2-5-9(11)6-3-8/h2-7,11H,1H3/b7-4+

InchiKey: NITWSHWHQAQBAW-QPJJXVBHSA-N

Formula: C10H10O3

SMILES: COC(=O)C=Cc1ccc(O)cc1

Mol. weight [g/mol]: 178.18

CAS: 3943-97-3

Physical Properties

Property code	Value	Unit	Source
gf	-162.59	kJ/mol	Joback Method
hf	-318.09	kJ/mol	Joback Method
hfus	30.22	kJ/mol	Solubilities of Cinnamic Acid Esters in Organic Solvents
hfus	30.22	kJ/mol	Solubilities of Cinnamic Acid Esters in Ionic Liquids
hvap	62.26	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.578		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
rinpol	1673.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1688.00		NIST Webbook
tb	615.95	K	Joback Method
tc	849.16	K	Joback Method
tf	407.68	K	Joback Method

vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.29	J/mol×K	615.95	Joback Method
cpg	378.94	J/mol×K	810.29	Joback Method
cpg	370.29	J/mol×K	771.43	Joback Method
cpg	361.09	J/mol×K	732.56	Joback Method
cpg	351.25	J/mol×K	693.69	Joback Method
cpg	340.68	J/mol×K	654.82	Joback Method
cpg	387.11	J/mol×K	849.16	Joback Method
dvisc	0.0000267	Pa×s	615.95	Joback Method
dvisc	0.0000399	Pa×s	581.24	Joback Method
dvisc	0.0000628	Pa×s	546.53	Joback Method
dvisc	0.0001050	Pa×s	511.82	Joback Method
dvisc	0.0001891	Pa×s	477.10	Joback Method
dvisc	0.0003738	Pa×s	442.39	Joback Method
dvisc	0.0008298	Pa×s	407.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3943973&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of cinnamic acid esters in binary mixtures of ionic liquids and organic solvents:	https://www.doi.org/10.1016/j.fluid.2010.05.015
Solubilities of Cinnamic Acid Esters in Ionic Liquids:	https://www.doi.org/10.1021/je800596c
Solubilities of Cinnamic Acid Esters in Organic Solvents:	https://www.doi.org/10.1021/je9004382
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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