2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, methyl ester

Other names: Cinnamic acid, 4-hydroxy-3-methoxy-, methyl ester
Ferulic acid methyl ester
Methyl ferulate
Methyl (2E)-3-(4-hydroxy-3-methoxyphenyl)-2-propenoate
Methyl 4'-hydroxy-3'-methoxycinnamate (methyl ferulate)

Inchi: InChI=1S/C11H12O4/c1-14-10-7-8(3-5-9(10)12)4-6-11(13)15-2/h3-7,12H,1-2H3/b6-4+

InchiKey: AUJXJFHANFIVKH-GQCTYLIASA-N

Formula: C11H12O4

SMILES: COC(=O)C=Cc1ccc(O)c(OC)c1

Mol. weight [g/mol]: 208.21

CAS: 2309-07-1

Physical Properties

Property code	Value	Unit	Source
gf	-268.80	kJ/mol	Joback Method
hf	-482.42	kJ/mol	Joback Method
hfus	27.86	kJ/mol	Joback Method
hvap	67.56	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.587		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	1854.80		NIST Webbook
tb	666.23	K	Joback Method
tc	892.63	K	Joback Method
tf	453.70	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.29	J/mol×K	892.63	Joback Method
cpg	399.15	J/mol×K	666.23	Joback Method
cpg	410.95	J/mol×K	703.96	Joback Method

cpg	422.02	J/mol×K	741.70	Joback Method
cpg	432.44	J/mol×K	779.43	Joback Method
cpg	442.25	J/mol×K	817.16	Joback Method
cpg	451.51	J/mol×K	854.90	Joback Method
dvisc	0.0000147	Pa×s	666.23	Joback Method
dvisc	0.0003045	Pa×s	453.70	Joback Method
dvisc	0.0001531	Pa×s	489.12	Joback Method
dvisc	0.0000845	Pa×s	524.54	Joback Method
dvisc	0.0000502	Pa×s	559.97	Joback Method
dvisc	0.0000318	Pa×s	595.39	Joback Method
dvisc	0.0000212	Pa×s	630.81	Joback Method
hfust	25.84	kJ/mol	335.70	NIST Webbook

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=C2309071&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

hfust: Enthalpy of fusion at a given temperature

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