Methyl 4-hydroxy-3,5-dimethoxycinnamate (methyl sinapate)

Other names: 3,5-dimethoxy-4-hydroxy cinnamic acid methyl ester
Inchi: InChI=1S/C12H14O5/c1-15-9-6-8(4-5-11(13)17-3)7-10(16-2)12(9)14/h4-7,14H,1-3H3/b5-
InchiKey: JHLPYWLKSLVYOI-SNAWJCMRSA-N
Formula: C12H14O5
SMILES: COC(=O)C=Cc1cc(OC)c(O)c(OC)c1
Mol. weight [g/mol]: 238.24
CAS: 20733-94-2

Physical Properties

Property code	Value	Unit	Source
gf	-375.01	kJ/mol	Joback Method
hf	-646.75	kJ/mol	Joback Method
hfus	29.86	kJ/mol	Solubilities of Cinnamic Acid Esters in Organic Solvents
hfus	29.86	kJ/mol	Solubilities of Cinnamic Acid Esters in Ionic Liquids
hvap	72.85	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.596		Crippen Method
mcvol	176.930	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	2092.10		NIST Webbook
tb	716.51	K	Joback Method
tc	937.06	K	Joback Method
tf	499.72	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.30	J/mol×K	716.51	Joback Method
cpg	484.50	J/mol×K	753.27	Joback Method
cpg	496.01	J/mol×K	790.03	Joback Method
cpg	506.86	J/mol×K	826.78	Joback Method

cpg	517.09	J/mol×K	863.54	Joback Method
cpg	526.73	J/mol×K	900.30	Joback Method
cpg	535.81	J/mol×K	937.06	Joback Method
dvisc	0.0001238	Pa×s	499.72	Joback Method
dvisc	0.0000677	Pa×s	535.85	Joback Method
dvisc	0.0000399	Pa×s	571.98	Joback Method
dvisc	0.0000251	Pa×s	608.12	Joback Method
dvisc	0.0000166	Pa×s	644.25	Joback Method
dvisc	0.0000115	Pa×s	680.38	Joback Method
dvisc	0.0000082	Pa×s	716.51	Joback Method
hfust	29.85	kJ/mol	361.80	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20733942&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
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