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

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/b5-4+

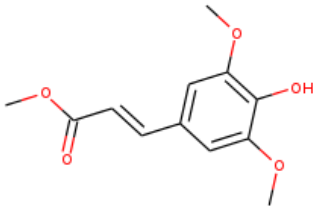
InChI Key: JHLPYWLKSLVYOI-SNAWJCMRSA-N

Formula: C12H14O5

SMILES: COC(=O)C=Cc1cc(OC)c(O)c(OC)c1

Molecular Weight: 238.24

CAS: 20733-94-2



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-375.01	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-646.75	kJ/mol	Joback Method
$\Delta_{fus} H°$	31.25	kJ/mol	Joback Method
$\Delta_{vap} H°$	72.85	kJ/mol	Joback Method
$logP_{oct/wat}$	1.60		Crippen Method
P_c	2902.98	kPa	Joback Method
T_{boil}	716.51	K	Joback Method
T_c	937.06	K	Joback Method
T_{fus}	499.72	K	Joback Method
V_c	0.61	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	472.30	J/mol×K	716.51	Joback Method
η	0.00	Pa×s	716.51	Joback Method
$\Delta_{fus} H$	29.85	kJ/mol	361.8	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/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/b5-4+
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H}$: Enthalpy of fusion at a given temperature (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).