2,3,4-Trimethoxycinnamic acid

Other names: 2-Propenoic acid, 3-(2,3,4-trimethoxyphenyl)-; trans-2,3,4-trimethoxycinnamic acid.

InChI: InChI=1S/C12H14O5/c1-15-9-6-4-8(5-7-10(13)14)11(16-2)12(9)17-3/h4-7H,1-3H3,(H,13,14)/b7-5+

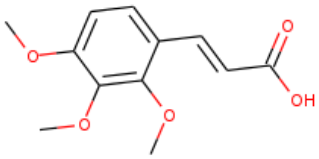
InChI Key: ZYOPDNLIHHFGEC-FNORWQNLSA-N

Formula: C12H14O5

SMILES: COc1ccc(C=CC(=O)O)c(OC)c1OC

Molecular Weight: 238.24

CAS: 33130-03-9



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-366.84	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-633.14	kJ/mol	Joback Method
$\Delta_{fus} H°$	29.16	kJ/mol	Joback Method
$\Delta_{vap} H°$	77.18	kJ/mol	Joback Method
$logP_{oct/wat}$	1.81		Crippen Method
P_c	2690.21	kPa	Joback Method
T_{boil}	733.05	K	Joback Method
T_c	933.80	K	Joback Method
T_{fus}	461.34	K	Joback Method
V_c	0.66	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	473.43	J/mol×K	733.05	Joback Method
η	0.00	Pa×s	733.05	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H14O5/c1-15-9-6-4-8(5-7-10(13)14)11(16-2)12(9)17-3/h4-7H,1-3H3,(H,13,14)/b7-5+
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).
$\Delta_{vap}\mathbf{H°}$: 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).