

trans-2,4-Dimethoxycinnamic acid, methyl ester

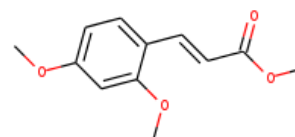
InChI: InChI=1S/C12H14O4/c1-14-10-6-4-9(11(8-10)15-2)5-7-12(13)16-3/h4-8H,1-3H3/b7-5+

InChI Key: OPFJHFOFMZFPKX-FNORWQNLSA-N

Formula: C12H14O4

SMILES: COC(=O)C=Cc1ccc(OC)cc1OC

Molecular Weight: 222.24



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-220.39	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-469.44	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	25.46	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	59.84	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.89		Crippen Method
P_c	2487.55	kPa	Joback Method
T_{boil}	635.89	K	Joback Method
T_c	847.87	K	Joback Method
T_{fus}	388.00	K	Joback Method
V_c	0.64	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	422.99	J/mol×K	635.89	Joback Method
η	0.00	Paxs	635.89	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H14O4/c1-14-10-6-4-9\(11\(8-10\)15-2\)5-7-12\(13\)16-3/h4-8H,1-3H3/b7-5+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H14O4/c1-14-10-6-4-9(11(8-10)15-2)5-7-12(13)16-3/h4-8H,1-3H3/b7-5+)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/molxK).

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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