

3,4-Dimethoxybenzylideneacetone

Other names: 3-Buten-2-one, 4-(3,4-dimethoxyphenyl)-;
4-(3,4-Dimethoxyphenyl)-3-buten-2-one.

InChI: InChI=1S/C12H14O3/c1-9(13)4-5-10-6-7-11(14-2)12(8-10)15-3/h4-8H,1-3H3/b5-4+

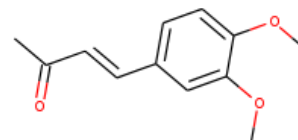
InChI Key: XUYBNDHXZMIALN-SNAWJCMRSA-N

Formula: C12H14O3

SMILES: COc1ccc(C=CC(C)=O)cc1OC

Molecular Weight: 206.24

CAS: 15001-27-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-115.39	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-337.22	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	24.28	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	57.43	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.31		Crippen Method
P_c	2530.27	kPa	Joback Method
T_{boil}	613.47	K	Joback Method
T_c	827.88	K	Joback Method
T_{fus}	365.77	K	Joback Method
V_c	0.62	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	398.09	J/mol×K	613.47	Joback Method
η	0.00	Paxs	613.47	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H14O3/c1-9\(13\)4-5-10-6-7-11\(14-2\)12\(8-10\)15-3/h4-8H,1-3H3/b5-4+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H14O3/c1-9(13)4-5-10-6-7-11(14-2)12(8-10)15-3/h4-8H,1-3H3/b5-4+)

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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