

Benzoic acid, 4-methyl-, phenyl ester

Other names: p-Toluic acid, phenyl ester; p-Toluylic acid, phenyl ester.

InChI: InChI=1S/C14H12O2/c1-11-7-9-12(10-8-11)14(15)16-13-5-3-2-4-6-13/h2-10H,1H3

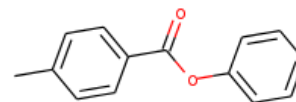
InChI Key: WOHDXQQIBMRFA-UHFFFAOYSA-N

Formula: C14H12O2

SMILES: Cc1ccc(C(=O)Oc2ccccc2)cc1

Molecular Weight: 212.24

CAS: 1900-85-2



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	48.27	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-115.50	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	22.50	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	61.13	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.214		Crippen Method
P_c	2862.74	kPa	Joback Method
T_{boil}	654.35	K	Joback Method
T_c	898.02	K	Joback Method
T_{fus}	385.06	K	Joback Method
V_c	0.627	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	415.01	J/mol×K	654.35	Joback Method
η	0.0001498	Paxs	654.35	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H12O2/c1-11-7-9-12\(10-8-11\)14\(15\)16-13-5-3-2-4-6-13/h2-10H,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H12O2/c1-11-7-9-12(10-8-11)14(15)16-13-5-3-2-4-6-13/h2-10H,1H3)

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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