Benzoic acid, 2-(4-methylbenzoyl)-

Other names: 2-(4-Methylbenzoyl)benzoic acid; 2-(p-Toluoyl)benzoic acid; 2-(p-Toluyl)benzoic acid; 4'-Methylbenzophenone-2-carboxylic acid; Benzoic acid, o-(p-toluoyl)-; o-(p-Toluoyl)benzoic acid; p-Toluoyl-o-benzoic acid.

InChI: InChI=1S/C15H12O3/c1-10-6-8-11(9-7-10)14(16)12-4-2-3-5-13(12)15(17)18/h2-9H,1H3,(H,17,18)

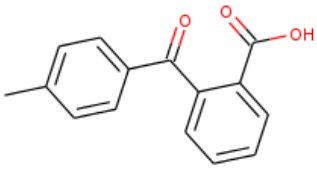
InChI Key: ICQOWIXIHDDXDI-UHFFFAOYSA-N

Formula: C15H12O3

SMILES: Cc1ccc(C(=O)c2ccccc2C(=O)O)cc1

Molecular Weight: 240.25

CAS: 85-55-2



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-113.68	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-280.20	kJ/mol	Joback Method
$\Delta_{fus} H°$	29.20	kJ/mol	Joback Method
$\Delta_{vap} H°$	85.03	kJ/mol	Joback Method
$logP_{oct/wat}$	2.92		Crippen Method
P_c	3059.17	kPa	Joback Method
T_{boil}	805.84	K	Joback Method
T_c	1035.00	K	Joback Method
T_{fus}	413.17 ± 0.30	K	NIST Webbook
T_{fus}	413.45 ± 0.20	K	NIST Webbook
V_c	0.69	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	501.16	J/mol×K	805.84	Joback Method
η	0.00	Pa×s	805.84	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H12O3/c1-10-6-8-11(9-7-10)14(16)12-4-2-3-5-13(12)15(17)18/h2-9H,1H3,(H,17,18)
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*P$_{oct/wat}$**: 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 (m^3/kg-mol).