

1,2-Benzenedicarboxylic acid, 4-methyl-

Other names: 4-Methyl-1,2-benzenedicarboxylic acid; 4-Methylphthalic acid; Phthalic acid, 4-methyl-

InChI: InChI=1S/C9H8O4/c1-5-2-3-6(8(10)11)7(4-5)9(12)13/h2-4H,1H3,(H,10,11)(H,12,13)

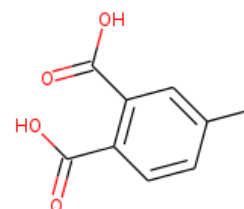
InChI Key: CWJJAFQCTXFSTA-UHFFFAOYSA-N

Formula: C₉H₈O₄

SMILES: Cc1ccc(C(=O)O)c(C(=O)O)c1

Molecular Weight: 180.16

CAS: 4316-23-8



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-413.43	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-545.12	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	23.70	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	86.08	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.39		Crippen Method
P_c	4621.41	kPa	Joback Method
T_{boil}	734.06	K	Joback Method
T_c	934.41	K	Joback Method
T_{fus}	464.15	K	Joback Method
V_c	0.48	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	329.42	J/mol×K	734.06	Joback Method
η	0.00	Paxs	734.06	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H8O4/c1-5-2-3-6\(8\(10\)11\)7\(4-5\)9\(12\)13/h2-4H,1H3,\(H,10,11\)\(H,12,13\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H8O4/c1-5-2-3-6(8(10)11)7(4-5)9(12)13/h2-4H,1H3,(H,10,11)(H,12,13))

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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