

3-Hydroxy-4-methylbenzoic acid

Other names: 3,4-Cresotic acid; 3-hydroxy-p-toluic acid; Benzoic acid, 3-hydroxy-4-methyl-

InChI:

InChI=1S/C8H8O3/c1-5-2-3-6(8(10)11)4-7(5)9/h2-4,9H,1H3,(H,10,11)

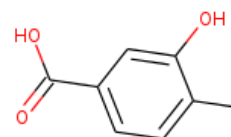
InChI Key: ZQLCWPXBHUALQC-UHFFFAOYSA-N

Formula: C₈H₈O₃

SMILES: Cc1ccc(C(=O)O)cc1O

Molecular Weight: 152.15

CAS: 586-30-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-301.10	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-425.51	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	21.60	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	72.78	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.399		Crippen Method
P_c	5359.18	kPa	Joback Method
T_{boil}	640.77	K	Joback Method
T_c	858.15	K	Joback Method
T_{fus}	441.33	K	Joback Method
V_c	0.366	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	276.61	J/mol×K	640.77	Joback Method
η	0.0000116	Paxs	640.77	Joback Method

Sources

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

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H8O3/c1-5-2-3-6\(8\(10\)11\)4-7\(5\)9/h2-4,9H,1H3,\(H,10,11\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H8O3/c1-5-2-3-6(8(10)11)4-7(5)9/h2-4,9H,1H3,(H,10,11))

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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