

4-Hydroxy-3-methylbenzaldehyde

Other names: Benzaldehyde, 4-hydroxy-3-methyl-

InChI: InChI=1S/C8H8O2/c1-6-4-7(5-9)2-3-8(6)10/h2-5,10H,1H3

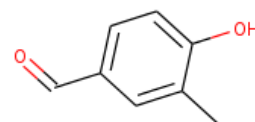
InChI Key: BAKYASSDAXQKKY-UHFFFAOYSA-N

Formula: C8H8O2

SMILES: Cc1cc(C=O)ccc1O

Molecular Weight: 136.15

CAS: 15174-69-3



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-134.88	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-246.28	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	18.20	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	56.07	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.51		Crippen Method
P_c	4775.98	kPa	Joback Method
T_{boil}	523.70	K	NIST Webbook
T_{boil}	413.20	K	NIST Webbook
T_c	774.17	K	Joback Method
T_{fus}	372.58	K	Joback Method
V_c	0.36	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	238.56	J/molxK	543.38	Joback Method
η	0.00	Paxs	543.38	Joback Method

Sources

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

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H8O2/c1-6-4-7\(5-9\)2-3-8\(6\)10/h2-5,10H,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H8O2/c1-6-4-7(5-9)2-3-8(6)10/h2-5,10H,1H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).

η : Dynamic viscosity (Pa×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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