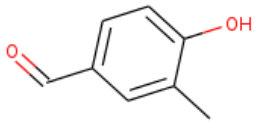
4-Hydroxy-3-methylbenzaldehyde

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
$\Delta_f G°$	-134.88	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-246.28	kJ/mol	Joback Method
$\Delta_{fus} H°$	18.20	kJ/mol	Joback Method
$\Delta_{vap} H°$	56.07	kJ/mol	Joback Method
$logP_{oct/wat}$	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
$C_{p,gas}$	238.56	J/mol×K	543.38	Joback Method
η	0.00	Pa×s	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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).