

Phenol, 4-butoxy-

Other names: 4-Butoxyphenol; Phenol, p-butoxy-; p-Butoxyphenol.

InChI: InChI=1S/C10H14O2/c1-2-3-8-12-10-6-4-9(11)5-7-10/h4-7,11H,2-3,8H2,1H3

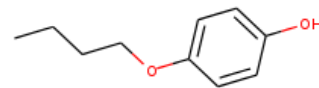
InChI Key: MBGGFXOXUIDRJD-UHFFFAOYSA-N

Formula: C10H14O2

SMILES: CCCCOC1=CC=C(O)C=C1

Molecular Weight: 166.22

CAS: 122-94-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-113.89	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-322.73	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	22.67	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	55.55	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.57		Crippen Method
P_c	3399.94	kPa	Joback Method
T_{boil}	557.92	K	Joback Method
T_c	773.80	K	Joback Method
T_{fus}	362.83	K	Joback Method
V_c	0.47	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	335.47	J/mol×K	557.92	Joback Method
η	0.00	Paxs	557.92	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H14O2/c1-2-3-8-12-10-6-4-9\(11\)5-7-10/h4-7,11H,2-3,8H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H14O2/c1-2-3-8-12-10-6-4-9(11)5-7-10/h4-7,11H,2-3,8H2,1H3)

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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