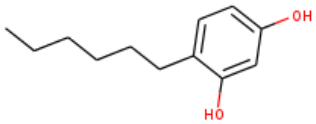
Hexylresorcinol



Other names: 1,3-Benzenediol, 4-hexyl-; 1,3-Dihydroxy-4-Hexylbenzene; 1,3-Dihydroxy-4-n-hexylbenzene; 1-(2',4'-Dihydroxyphenyl)hexane; 4-(1-Hexyl)resorcinol; 4-Hexyl-1,3-benzenediol; 4-Hexyl-1,3-dihydroxybenzene; 4-Hexylresorcine; 4-Hexylresorcinol; 4-n-Hexylresorcinol; Adrover; Antascarin; Ascaricid; Ascarinol; Ascaryl; Caprokol; Crystoids; Cystoids Anthelmintic; Gelovermin; Hexylresorcin; Hidesol; Mycoderm; NCI-C55787; NSC 1570; Oxana; Prensol; Resorcinol, 4-hexyl-; S.T. 37; ST-37; Sucrets; Worm-agen; p-Hexylresorcinol.

InChI: InChI=1S/C12H18O2/c1-2-3-4-5-6-10-7-8-11(13)9-12(10)14/h7-9,13-14H,2-6H2,1H3

InChI Key: WFJIVOKAWHGMBH-UHFFFAOYSA-N

Formula: C12H18O2

SMILES: CCCCCCc1ccc(O)cc1O

Molecular Weight: 194.27

CAS: 136-77-6

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-146.67	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-409.10	kJ/mol	Joback Method
$\Delta_{fus} H°$	32.44	kJ/mol	Joback Method
$\Delta_{vap} H°$	70.61	kJ/mol	Joback Method
$logP_{oct/wat}$	3.22		Crippen Method
P_c	3299.15	kPa	Joback Method
T_{boil}	607.20	K	NIST Webbook
T_{boil}	452.20	K	NIST Webbook
T_c	882.46	K	Joback Method
T_{fus}	341.00 ± 0.10	K	NIST Webbook
V_c	0.53	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	458.64	J/mol×K	661.88	Joback Method
η	0.00	Pa×s	661.88	Joback Method
$\Delta_{fus}H$	19.04	kJ/mol	341.5	NIST Webbook
$\Delta_{fus}H$	19.04	kJ/mol	341.5	NIST Webbook
$\Delta_{vap}H$	88.10	kJ/mol	464.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H18O2/c1-2-3-4-5-6-10-7-8-11(13)9-12(10)14/h7-9,13-14H,2-6H2,1H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°$_{gas}$**: Enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{fus}**H**: Enthalpy of fusion at a given temperature (kJ/mol).
Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (kJ/mol).
Δ_{vap}**H**: Enthalpy of vaporization at a given temperature (kJ/mol).
***log*P$_{oct/wat}$**: 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 (m^3/kg-mol).