Phenol, 2-(1-ethylbutyl)-6-nitro

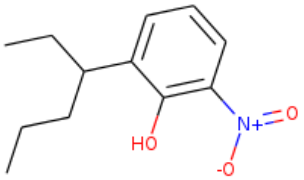
InChI: InChI=1S/C12H17NO3/c1-3-6-9(4-2)10-7-5-8-11(12(10)14)13(15)16/h5,7-9,14H,3-4,6H2,1-2H3

InChI Key: OXKMZSZQCOKAFN-UHFFFAOYSA-N

Formula: C12H17NO3

SMILES: CCCC(CC)c1cccc([N+](=O)[O-])c1O

Molecular Weight: 223.27



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	31.43	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-259.30	kJ/mol	Joback Method
$\Delta_{fus} H°$	34.11	kJ/mol	Joback Method
$\Delta_{vap} H°$	74.46	kJ/mol	Joback Method
$logP_{oct/wat}$	3.594		Crippen Method
P_c	2814.34	kPa	Joback Method
T_{boil}	737.64	K	Joback Method
T_c	975.34	K	Joback Method
T_{fus}	504.27	K	Joback Method
V_c	0.641	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	508.19	J/mol×K	737.64	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H17NO3/c1-3-6-9(4-2)10-7-5-8-11(12(10)14)13(15)16/h5,7-9,14H,3-4,6H2,1-2H3

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f\mathbf{G°}$: 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).