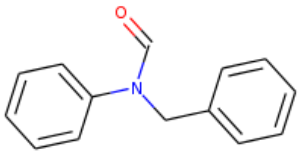
Formanilide, n-benzyl-

InChI: InChI=1S/C14H13NO/c16-12-15(14-9-5-2-6-10-14)11-13-7-3-1-4-8-13/h1-10,12H,11H2
InChI Key: CEIHCMMUIHDOQQ-UHFFFAOYSA-N
Formula: C14H13NO
SMILES: O=CN(Cc1ccccc1)c1ccccc1
Molecular Weight: 211.26
CAS: 16350-99-5



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	303.08	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	122.72	kJ/mol	Joback Method
$\Delta_{fus} H°$	25.41	kJ/mol	Joback Method
$\Delta_{vap} H°$	60.07	kJ/mol	Joback Method
$logP_{oct/wat}$	2.850		Crippen Method
P_c	2992.59	kPa	Joback Method
T_{boil}	634.18	K	Joback Method
T_c	871.27	K	Joback Method
T_{fus}	374.85	K	Joback Method
V_c	0.638	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	428.61	J/mol×K	634.18	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H13NO/c16-12-15(14-9-5-2-6-10-14)11-13-7-3-1-4-8-13/h1-10,12H,11H2

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: 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).

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