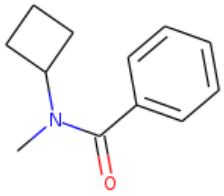
N-cyclobutyl-N-methyl-benzamide

InChI: InChI=1S/C12H15NO/c1-13(11-8-5-9-11)12(14)10-6-3-2-4-7-10/h2-4,6-7,11H,5,8-9H2,1H3
InChI Key: QAAGQIMSYFWKMD-UHFFFAOYSA-N
Formula: C12H15NO
SMILES: CN(C(=O)c1ccccc1)C1CCC1
Molecular Weight: 189.25



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	193.08	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-32.89	kJ/mol	Joback Method
$\Delta_{fus} H°$	21.53	kJ/mol	Joback Method
$\Delta_{vap} H°$	53.46	kJ/mol	Joback Method
$logP_{oct/wat}$	2.31		Crippen Method
P_c	3009.03	kPa	Joback Method
T_{boil}	577.96	K	Joback Method
T_c	806.14	K	Joback Method
T_{fus}	348.24	K	Joback Method
V_c	0.57	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	391.20	J/mol×K	577.96	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H15NO/c1-13(11-8-5-9-11)12(14)10-6-3-2-4-7-10/h2-4,6-7,11H,5,8-9H2,1H3

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).