Benzenamine, 2,4,6-tris(1,1-dimethylethyl)-

Other names: 2,4,6-tri-t-Butylaniline; 2,4,6-tri-tert-Butylaniline; Aniline, 2,4,6-tri-tert-butyl-; Aniline, tri-tert-butyl-.

InChI: InChI=1S/C18H31N/c1-16(2,3)12-10-13(17(4,5)6)15(19)14(11-12)18(7,8)9/h10-11H,19H2,1-9H3

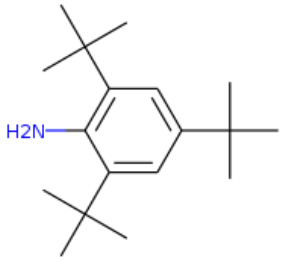
InChI Key: REJGDSCBQPJPQT-UHFFFAOYSA-N

Formula: C18H31N

SMILES: CC(C)(C)c1cc(C(C)(C)C)c(N)c(C(C)(C)C)c1

Molecular Weight: 261.45

CAS: 961-38-6



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	259.17	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-205.19	kJ/mol	Joback Method
$\Delta_{fus} H°$	18.21	kJ/mol	Joback Method
$\Delta_{sub} H°$	92.50 ± 1.10	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	66.68	kJ/mol	Joback Method
IE	6.90	eV	NIST Webbook
IE	7.30	eV	NIST Webbook
$logP_{oct/wat}$	5.16		Crippen Method
P_c	1542.71	kPa	Joback Method
T_{boil}	715.70	K	Joback Method
T_c	941.27	K	Joback Method
T_{fus}	447.12	K	Joback Method
V_c	0.93	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	736.39	J/mol×K	715.7	Joback Method
$\Delta_{fus}H$	19.38	kJ/mol	426.4	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H31N/c1-16(2,3)12-10-13(17(4,5)6)15(19)14(11-12)18(7,8)9/h10-11H,19H2,1-9H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{fus} H$: Enthalpy of fusion at a given temperature (kJ/mol).
$\Delta_{sub} H°$: Enthalpy of sublimation at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
IE: Ionization energy (eV).
***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).