1-Octanamine

Other names: 1-Aminooctane; 1-Octylamine; Amine 8D; Armeen 8; Caprylamine; Caprylylamine; Monoctylamine; Monooctylamine; NSC 9824; Octanamine; Octylamine; n-C8H17NH2; n-Octylamine; n-Octylamine, mono-.

InChI: InChI=1S/C8H19N/c1-2-3-4-5-6-7-8-9/h2-9H2,1H3

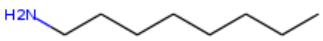
InChI Key: IOQPZZOEVPZRBK-UHFFFAOYSA-N

Formula: C8H19N

SMILES: CCCCCCCCN

Molecular Weight: 129.24

CAS: 111-86-4



Physical Properties

Property	Value	Unit	Source
PAff	928.90	kJ/mol	NIST Webbook
PAff	925.10	kJ/mol	NIST Webbook
PAff	924.70	kJ/mol	NIST Webbook
BasG	895.00	kJ/mol	NIST Webbook
BasG	879.50 ± 9.20	kJ/mol	NIST Webbook
$\Delta_c H°_{liquid}$	-5635.38 ± 0.96	kJ/mol	NIST Webbook
$\Delta_f G°$	82.93	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-173.50 ± 1.30	kJ/mol	NIST Webbook
$\Delta_f H°_{liquid}$	-228.10 ± 1.20	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	21.67	kJ/mol	Joback Method
$\Delta_{vap} H°$	54.63 ± 0.96	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	54.60	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	54.80 ± 0.50	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	54.60	kJ/mol	NIST Webbook
IE	8.50	eV	NIST Webbook
$logP_{oct/wat}$	2.31		Crippen Method
P_c	2617.00 ± 400.00	kPa	NIST Webbook

Property	Value	Unit	Source
T_{boil}	449.20	K	NIST Webbook
T_{boil}	452.80	K	NIST Webbook
T_{boil}	452.75 ± 1.00	K	NIST Webbook
T_{boil}	452.00 ± 2.00	K	NIST Webbook
T_{boil}	452.15 ± 1.00	K	NIST Webbook
T_{boil}	451.65 ± 3.00	K	NIST Webbook
T_{boil}	452.65 ± 3.00	K	NIST Webbook
T_{boil}	445.65 ± 5.00	K	NIST Webbook
T_{boil}	459.15 ± 6.00	K	NIST Webbook
T_{c}	641.00 ± 3.00	K	NIST Webbook
T_{fus}	272.75 ± 0.20	K	NIST Webbook
T_{fus}	273.15 ± 0.50	K	NIST Webbook
T_{fus}	272.15 ± 0.50	K	NIST Webbook
V_{c}	0.51	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	292.59	J/mol×K	454.97	Joback Method
$C_{p,liquid}$	309.30	J/mol×K	298.15	NIST Webbook
$\Delta_{vap}H$	50.80	kJ/mol	380.5	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H19N/c1-2-3-4-5-6-7-8-9/h2-9H2,1H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

PAff: Proton affinity (kJ/mol).

BasG: Gas basicity (kJ/mol).

Δ_c**H°**$_{liquid}$: Standard liquid enthalpy of combustion (kJ/mol).

C$_{p,gas}$: Ideal gas heat capacity (J/mol×K).

C$_{p,liquid}$: Liquid phase heat capacity (J/mol×K).

Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).

Δ_f**H°**$_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

Δ_f**H°**$_{liquid}$: Liquid phase enthalpy of formation at standard conditions (kJ/mol).

Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (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).

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).