1-Undecanol

Other names: 1-Hendecanol; 1-Undecyl alcohol; Alcohol c-11; Decyl carbinol; Hendecanoic alcohol; Hendecyl alcohol; NSC 403667; Neodol 1; Tip-Nip; Undecan-1-ol; Undecanol; Undecanol-(1); Undecyl alcohol; n-Hendecylenic alcohol; n-Undecan-1-ol; n-Undecanol; n-Undecyl alcohol.

InChI:
InChI=1S/C11H24O/c1-2-3-4-5-6-7-8-9-10-11-12/h12H,2-11H2,1H3

InChI Key: KJIOQYGWTQBHNH-UHFFFAOYSA-N

Formula: C11H24O

SMILES: CCCCCCCCCCCO

Molecular Weight: 172.31

CAS: 112-42-5

Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{liquid}$	-7253.70 ± 0.80	kJ/mol	NIST Webbook
$\Delta_f G°$	-95.08	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-422.60	kJ/mol	Joback Method
$\Delta_f H°_{liquid}$	-504.90 ± 0.80	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	28.33	kJ/mol	Joback Method
$\Delta_{vap} H°$	85.80 ± 2.10	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	84.70	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	83.50	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	86.80	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	85.60	kJ/mol	NIST Webbook
$logP_{oct/wat}$	3.51		Crippen Method
P_c	2150.00 ± 50.00	kPa	NIST Webbook
P_c	2147.00 ± 30.00	kPa	NIST Webbook
P_c	2147.00 ± 30.00	kPa	NIST Webbook
T_{boil}	419.20	K	NIST Webbook
T_{boil}	404.20	K	NIST Webbook
T_c	703.60 ± 1.50	K	NIST Webbook

Property	Value	Unit	Source
T_c	704.20	K	NIST Webbook
T_c	703.00 ± 0.80	K	NIST Webbook
T_c	704.20 ± 2.40	K	NIST Webbook
T_c	703.00 ± 0.80	K	NIST Webbook
T_c	703.38	K	NIST Webbook
T_{fus}	288.45 ± 0.50	K	NIST Webbook
T_{fus}	289.65 ± 0.30	K	NIST Webbook
V_c	0.72	m^3/kg-mol	NIST Webbook

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	428.64	J/mol×K	543.26	Joback Method
$C_{p,liquid}$	406.34	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	419.80	J/mol×K	303.0	NIST Webbook
$C_{p,liquid}$	406.80	J/mol×K	303.15	NIST Webbook
$C_{p,liquid}$	414.80	J/mol×K	303.65	NIST Webbook
η	0.00	Pa×s	543.26	Joback Method
$\Delta_{vap}H$	83.60	kJ/mol	317.5	NIST Webbook
$\Delta_{vap}H$	79.50	kJ/mol	333.5	NIST Webbook
$\Delta_{vap}H$	72.30	kJ/mol	454.5	NIST Webbook
$\Delta_{vap}H$	68.70	kJ/mol	458.0	NIST Webbook
$\Delta_{vap}H$	68.50	kJ/mol	463.5	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H24O/c1-2-3-4-5-6-7-8-9-10-11-12/h12H,2-11H2,1H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\Delta_c H°_{liquid}$: 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).
η: Dynamic viscosity (Pa×s).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_f H°_{liquid}$: Liquid phase enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\Delta_{vap} H$: Enthalpy of vaporization at a given temperature (kJ/mol).
$logP_{oct/wat}$: 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).