

(S)-9-methyldecan-3-ol

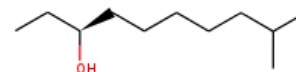
InChI: InChI=1S/C11H24O/c1-4-11(12)9-7-5-6-8-10(2)3/h10-12H,4-9H2,1-3H3/t11-/m1/s1

InChI Key: GVNZAPCZQSDLGP-LLVKDONJSA-N

Formula: C11H24O

SMILES: CCC(O)CCCCC(C)C

Molecular Weight: 172.31



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-99.96	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-433.16	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	21.29	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	55.98	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.36		Crippen Method
P_c	2131.49	kPa	Joback Method
T_{boil}	542.38	K	Joback Method
T_c	705.81	K	Joback Method
T_{fus}	244.55	K	Joback Method
V_c	0.66	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	429.18	J/mol×K	542.38	Joback Method
η	0.00	Paxs	542.38	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H24O/c1-4-11\(12\)9-7-5-6-8-10\(2\)3/h10-12H,4-9H2,1-3H3/t11-m/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H24O/c1-4-11(12)9-7-5-6-8-10(2)3/h10-12H,4-9H2,1-3H3/t11-m/s1)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/molxK).

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (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 (m³/kg-mol).

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