

8-dodecenal, E

Other names: (E)-8-Dodecenal.

InChI: InChI=1S/C12H22O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h4-5,12H,2-3,6-11H2,1H3/b5-4+

InChI Key: GDNSCKFMUMBMIC-SNAWJCMRSA-N

Formula: C12H22O

SMILES: CCCC=CCCCCCC=O

Molecular Weight: 182.30



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	30.86	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-259.37	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	29.33	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	48.98	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.882		Crippen Method
P_c	1985.89	kPa	Joback Method
T_{boil}	526.78	K	Joback Method
T_c	700.00	K	Joback Method
T_{fus}	261.92	K	Joback Method
V_c	0.705	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	418.84	J/mol×K	526.78	Joback Method
η	0.0002139	Paxs	526.78	Joback Method

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H22O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h4-5,12H,2-3,6-11H2,1H3/b5-4+>

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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