

1,3-Dioxane, 2-propyl-4-(2-pentenyl), 2R,4R

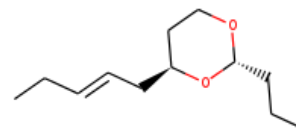
InChI: InChI=1S/C12H22O2/c1-3-5-6-8-11-9-10-13-12(14-11)7-4-2/h5-6,11-12H,3-4,7-10H2,1-2H3/b6-5+/t11-,12-/m0/s1

InChI Key: HUMNXQDSONGUJF-WTIVYXKASA-N

Formula: C12H22O2

SMILES: CCC=CCC1CCOC(CCC)O1

Molecular Weight: 198.30



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-25.12	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-403.81	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	35.90	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	51.40	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.274		Crippen Method
P_c	2135.43	kPa	Joback Method
T_{boil}	546.90	K	Joback Method
T_c	745.76	K	Joback Method
T_{fus}	276.20	K	Joback Method
V_c	0.661	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	449.13	J/mol×K	546.9	Joback Method
η	0.0002168	Paxs	546.9	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H22O2/c1-3-5-6-8-11-9-10-13-12\(14-11\)7-4-2/h5-6,11-12H,3-4,7-10H2,1-2H3/b6-5+/t11-,12-/m0/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H22O2/c1-3-5-6-8-11-9-10-13-12(14-11)7-4-2/h5-6,11-12H,3-4,7-10H2,1-2H3/b6-5+/t11-,12-/m0/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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