

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

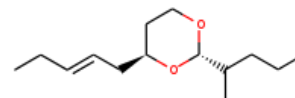
InChI: InChI=1S/C14H26O2/c1-4-6-7-9-13-10-11-15-14(16-13)12(3)8-5-2/h6-7,12-14H,4-5,8-11H2,1-3H3/b7-6+/t12?,13-,14-/m0/s1

InChI Key: HEZVGAKBJDMI EP-ASHKF XBZSA-N

Formula: C₁₄H₂₆O₂

SMILES: CCC=CCC1CCOC(C(C)CCC)O1

Molecular Weight: 226.35



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-10.72	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-450.37	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	37.56	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	55.47	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.911		Crippen Method
P_c	1813.86	kPa	Joback Method
T_{boil}	592.22	K	Joback Method
T_c	789.59	K	Joback Method
T_{fus}	283.74	K	Joback Method
V_c	0.767	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	553.65	J/mol×K	592.22	Joback Method
η	0.0001668	Paxs	592.22	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H26O2/c1-4-6-7-9-13-10-11-15-14\(16-13\)12\(3\)8-5-2/h6-7,12-14H,4-5,8-11H2,1-3H3/b7-6+/t12?,13-,14-/m0/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H26O2/c1-4-6-7-9-13-10-11-15-14(16-13)12(3)8-5-2/h6-7,12-14H,4-5,8-11H2,1-3H3/b7-6+/t12?,13-,14-/m0/s1)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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