1,3-Dioxane, 2-isopropyl-4-(2-pentenyl), 2S,4R

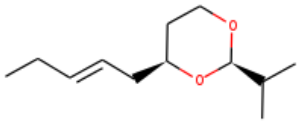
InChI: InChI=1S/C12H22O2/c1-4-5-6-7-11-8-9-13-12(14-11)10(2)3/h5-6,10-12H,4,7-9H2,1-3H3/b6-5+/t11-,12+/m0/s1

InChI Key: URODEFYSNWWYIU-CYLBZQBVSA-N

Formula: C12H22O2

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

Molecular Weight: 198.30



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-27.56	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-409.09	kJ/mol	Joback Method
$\Delta_{fus} H°$	32.38	kJ/mol	Joback Method
$\Delta_{vap} H°$	51.02	kJ/mol	Joback Method
$logP_{oct/wat}$	3.130		Crippen Method
P_c	2151.31	kPa	Joback Method
T_{boil}	546.46	K	Joback Method
T_c	749.53	K	Joback Method
T_{fus}	261.20	K	Joback Method
V_c	0.655	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	449.38	J/mol×K	546.46	Joback Method
η	0.0002037	Pa×s	546.46	Joback Method

Sources

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

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

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).