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

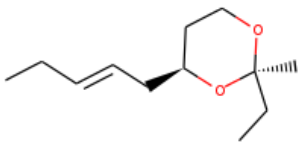
InChI: InChI=1S/C12H22O2/c1-4-6-7-8-11-9-10-13-12(3,5-2)14-11/h6-7,11H,4-5,8-10H2,1-3H3/b7-6+/t11-,12+/m0/s1

InChI Key: ZBHDHORAJVLHID-FNSAGKMKSA-N

Formula: C12H22O2

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

Molecular Weight: 198.30



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-30.61	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-388.57	kJ/mol	Joback Method
$\Delta_{fus} H°$	29.60	kJ/mol	Joback Method
$\Delta_{vap} H°$	50.25	kJ/mol	Joback Method
$log P_{oct/wat}$	3.274		Crippen Method
P_c	2227.09	kPa	Joback Method
T_{boil}	547.14	K	Joback Method
T_c	753.86	K	Joback Method
T_{fus}	300.10	K	Joback Method
V_c	0.659	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	448.38	J/mol×K	547.14	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H22O2/c1-4-6-7-8-11-9-10-13-12(3,5-2)14-11/h6-7,11H,4-5,8-10H2,1-3H3/b7-6+/t11-,12+/m0/s1

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*$P_{oct/wat}$**: 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 (m^3/kg-mol).