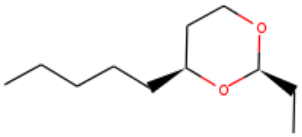
1,3-Dioxane, 2-ethyl-4-pentyl, 2S,4R

InChI: InChI=1S/C11H22O2/c1-3-5-6-7-10-8-9-12-11(4-2)13-10/h10-11H,3-9H2,1-2H3/t10-,11+/m0/s1
InChI Key: UCGYQTHBPZXKHC-WDEREUQCSA-N
Formula: C11H22O2
SMILES: CCCCCC1CCOC(CC)O1
Molecular Weight: 186.29



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-113.76	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-500.39	kJ/mol	Joback Method
$\Delta_{fus} H°$	33.11	kJ/mol	Joback Method
$\Delta_{vap} H°$	49.22	kJ/mol	Joback Method
$logP_{oct/wat}$	3.11		Crippen Method
P_c	2224.99	kPa	Joback Method
T_{boil}	519.86	K	Joback Method
T_c	712.81	K	Joback Method
T_{fus}	270.01	K	Joback Method
V_c	0.63	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	416.76	J/mol×K	519.86	Joback Method
η	0.00	Pa×s	519.86	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H22O2/c1-3-5-6-7-10-8-9-12-11(4-2)13-10/h10-11H,3-9H2,1-2H3/t10-,11+/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).

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