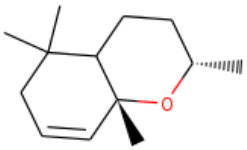
Dihydroedulan IA

InChI: InChI=1S/C13H22O/c1-10-6-7-11-12(2,3)8-5-9-13(11,4)14-10/h5,9-11H,6-8H2,1-4H3/t10-,11?,13+/m1/s1
InChI Key: IVTQSEFLDHBCDZ-XEEJXUNPSA-N
Formula: C13H22O
SMILES: CC1CCC2C(C)(C)CC=CC2(C)O1
Molecular Weight: 194.31
CAS: 74006-61-4



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	49.12	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-275.11	kJ/mol	Joback Method
$\Delta_{fus} H°$	16.04	kJ/mol	Joback Method
$\Delta_{vap} H°$	46.93	kJ/mol	Joback Method
$logP_{oct/wat}$	3.546		Crippen Method
P_c	2367.97	kPa	Joback Method
T_{boil}	544.65	K	Joback Method
T_c	774.56	K	Joback Method
T_{fus}	324.72	K	Joback Method
V_c	0.646	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	451.15	J/mol×K	544.65	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H22O/c1-10-6-7-11-12(2,3)8-5-9-13(11,4)14-10/h5,9-11H,6-8H2,1-4H3/t10-,11?,13+/m1/s1

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

Legend

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