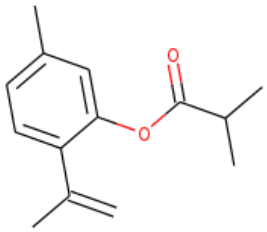
8,9-Dehydrothymyl isobutyrate

InChI: InChI=1S/C14H18O2/c1-9(2)12-7-6-11(5)8-13(12)16-14(15)10(3)4/h6-8,10H,1H2,2-5H3
InChI Key: BSAPRZRKFYAPEB-UHFFFAOYSA-N
Formula: C14H18O2
SMILES: C=C(C)c1ccc(C)cc1OC(=O)C(C)C
Molecular Weight: 218.29
CAS: 38146-79-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	3.08	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-253.14	kJ/mol	Joback Method
$\Delta_{fus} H°$	21.95	kJ/mol	Joback Method
$\Delta_{vap} H°$	58.54	kJ/mol	Joback Method
$logP_{oct/wat}$	3.59		Crippen Method
P_c	2143.35	kPa	Joback Method
T_{boil}	628.77	K	Joback Method
T_c	841.84	K	Joback Method
T_{fus}	340.44	K	Joback Method
V_c	0.71	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	471.75	J/mol×K	628.77	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H18O2/c1-9(2)12-7-6-11(5)8-13(12)16-14(15)10(3)4/h6-8,10H,1H2,2-5H3

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).