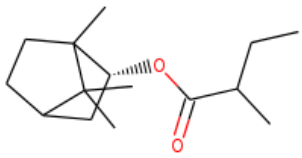
isobornyl2-methylbutanoate

InChI: InChI=1S/C15H26O2/c1-6-10(2)13(16)17-12-9-11-7-8-15(12,5)14(11,3)4/h10-12H,6-9H2,1-5H3/t10?,11?,12-,15?/m0/s1
InChI Key: CEVCMCWHMHJEQS-WAQQSHLVSA-N
Formula: C15H26O2
SMILES: CCC(C)C(=O)OC1CC2CCC1(C)C2(C)C
Molecular Weight: 238.37



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-77.94	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-473.77	kJ/mol	Joback Method
$\Delta_{fus} H°$	17.59	kJ/mol	Joback Method
$\Delta_{vap} H°$	54.83	kJ/mol	Joback Method
$logP_{oct/wat}$	3.79		Crippen Method
P_c	1898.60	kPa	Joback Method
T_{boil}	627.34	K	Joback Method
T_c	836.82	K	Joback Method
T_{fus}	387.65	K	Joback Method
V_c	0.79	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	593.55	J/mol×K	627.34	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H26O2/c1-6-10(2)13(16)17-12-9-11-7-8-15(12,5)14(11,3)4/h10-12H,6-9H2,1-5H3/t10?,11?,12-,15?/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).
$\mathbf{\Delta_f G°}$: 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).