

5-Camphenyl acetate

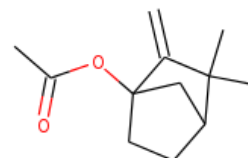
InChI: InChI=1S/C12H18O2/c1-8-11(3,4)10-5-6-12(8,7-10)14-9(2)13/h10
H,1,5-7H2,2-4H3

InChI Key: XCRWYCLRGYBKLG-UHFFFAOYSA-N

Formula: C12H18O2

SMILES: C=C1C(C)(C)C2CCC1(OC(C)=O)C2

Molecular Weight: 194.27



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-39.97	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-301.99	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	11.11	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	49.01	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.68		Crippen Method
P_c	2595.13	kPa	Joback Method
T_{boil}	562.97	K	Joback Method
T_c	780.60	K	Joback Method
T_{fus}	386.76	K	Joback Method
V_c	0.62	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	416.62	J/mol×K	562.97	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H18O2/c1-8-11\(3,4\)10-5-6-12\(8,7-10\)14-9\(2\)13/h10H,1,5-7H2,2-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H18O2/c1-8-11(3,4)10-5-6-12(8,7-10)14-9(2)13/h10H,1,5-7H2,2-4H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p, gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: 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 (m³/kg-mol).

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