

Marsupellyl acetate

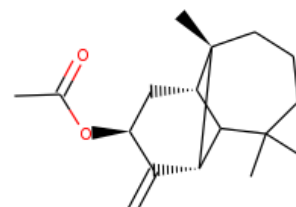
InChI: InChI=1S/C17H26O2/c1-10-13(19-11(2)18)9-12-15-14(10)17(12,5)8-6-7-16(15,3)4/h12-15H,1,6-9H2,2-5H3/t12-,13-,14-,15?,17-/m1/s1

InChI Key: RCEFXIVQCAIFDV-FQAZMDJZSA-N

Formula: C17H26O2

SMILES: C=C1C2C3C(CC1OC(C)=O)C2(C)CCCC3(C)C

Molecular Weight: 262.39



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	35.36	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-379.23	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	22.24	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	59.61	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.96		Crippen Method
P_c	1804.63	kPa	Joback Method
T_{boil}	679.04	K	Joback Method
T_c	899.33	K	Joback Method
T_{fus}	449.05	K	Joback Method
V_c	0.84	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	669.85	J/mol×K	679.04	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H26O2/c1-10-13\(19-11\(2\)18\)9-12-15-14\(10\)17\(12,5\)8-6-7-16\(15,3\)4/h12-15H,1,6-9H2,2-5H3/t12-,13-,14-,15?,17-/m1/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H26O2/c1-10-13(19-11(2)18)9-12-15-14(10)17(12,5)8-6-7-16(15,3)4/h12-15H,1,6-9H2,2-5H3/t12-,13-,14-,15?,17-/m1/s1)

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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