Methyl 5-.beta.-cholan-3-.alpha.,7-.alpha.-diol-12-one-24-oate

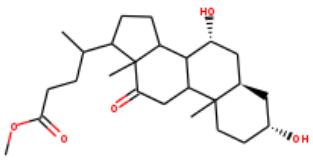
InChI: InChI=1S/C25H40O5/c1-14(5-8-22(29)30-4)17-6-7-18-23-19(13-21(28)25(17,18)3)24(2)10-9-16(26)11-15(24)12-20(23)27/h14-20,23,26-27H,5-13H2,1-4H3/t14?,15-,16-,17?,18?,19?,20-,23?,24?,25?/m0/s1

InChI Key: LGWDBNNCYKGKFM-ZGPVKVJISA-N

Formula: C25H40O5

SMILES: COC(=O)CCC(C)C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CC(=O)C12C

Molecular Weight: 420.58



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-340.00	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1062.39	kJ/mol	Joback Method
$\Delta_{fus} H°$	42.25	kJ/mol	Joback Method
$\Delta_{vap} H°$	114.28	kJ/mol	Joback Method
$logP_{oct/wat}$	3.75		Crippen Method
P_c	1298.60	kPa	Joback Method
T_{boil}	1124.87	K	Joback Method
T_c	1378.07	K	Joback Method
T_{fus}	699.29	K	Joback Method
V_c	1.28	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1427.29	J/mol×K	1124.87	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H40O5/c1-14(5-8-22(29)30-4)17-6-7-18-23-19(13-21(28)25(17,18)3)24(2)10-9-16(26)11-15(24)12-20(23)27/h14-20,23,26-27H,5-13H2,1-4H3/t14?,15-,16-,17?,18?,19?,20-,23?,24?,25?/m0/s1

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*$P_{oct/wat}$**: 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 (m^3/kg-mol).