5-«alpha»-Pregnane-3-«beta»,17-«alpha»,20-«alpha»-triol

InChI: InChI=1S/C21H36O3/c1-13(22)21(24)11-8-18-16-5-4-14-12-15(23)6-9-19(14,2)17(16)7-10-20(18,21)3/h13-18,22-24H,4-12H2,1-3H3/t13-,14-,15-,16?,17?,18?,19-,20-,21-/m1/s1

InChI Key: SCPADBBISMMJAW-NAJBNHQKSA-N

Formula: C21H36O3

SMILES: CC(O)C1(O)CCC2C3CCC4CC(O)CCC4(C)C3CCC21C

Molecular Weight: 336.51

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-151.77	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-713.98	kJ/mol	Joback Method
$\Delta_{fus} H°$	26.32	kJ/mol	Joback Method
$\Delta_{vap} H°$	107.81	kJ/mol	Joback Method
$logP_{oct/wat}$	3.50		Crippen Method
P_c	1887.08	kPa	Joback Method
T_{boil}	986.33	K	Joback Method
T_c	1209.67	K	Joback Method
T_{fus}	602.79	K	Joback Method
V_c	1.04	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1124.32	J/mol×K	986.33	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H36O3/c1-13(22)21(24)11-8-18-16-5-4-14-12-15(23)6-9-19(14,2)17(16)7-10-20(18,21)3/h13-18,22-24H,4-12H2,1-3H3/t13-,14-,15-,16?,17?,18?,19-,20-,21-/m1/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).