

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

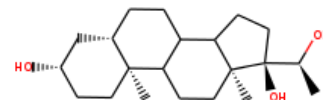
InChI: InChI=1S/C21H36O3/c1-13(22)21(24)11-8-18-16-5-4-14-12-15(23)
6-9-19(14,2)17(16)7-10-20(18,21)3/h13-18,22-24H,4-12H2,1-3H3/t13-,14-
,15-,16?,17?,18?,19-,20-,21-/m1/s1

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
$\Delta_f G^\circ$	-151.77	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-713.98	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	26.32	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	107.81	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	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
$C_{p,\text{gas}}$	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](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/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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