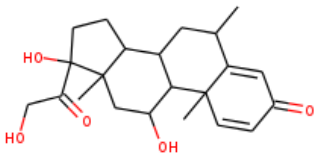
Methylprednisolone



Other names: (6«alpha»,11«beta»)-11,17,21-Trihydroxy-6-methylpregna-1,4-diene-3,20-dione; 1,4-Pregnadiene-3,20-dione, 11beta,17alpha,21-trihydroxy-6alpha-methyl-; 11-«beta»,17,21-Trihydroxy-6-«alpha»-methylpregna-1,4-diene-3,20-dione; 11-«beta»,17-«alpha»,21-Trihydroxy-6-«alpha»-methyl-1,4-pregnadiene-3,20-dione; 6-«alpha»-Methylprednisolone; A-Methapred; Besonia; Depo-Medrol; Dopomedrol; M-Prednisol; MEPRDL; Medesone; Medrate; Medrol; Medrol adt pak; Medrol dosepak; Medrone; Mesopren; Metastab; Metilbetasone; Metrisone; Moderin; NSC-19987; Noretona; Prednisolone, 6«alpha»-methyl-; Prednisolone, methyl-; Pregna-1,4-diene-3,20-dione, 11,17,21-trihydroxy-6-methyl-, (6«alpha»,11«beta»)-; Pregna-1,4-diene-3,20-dione, 11«beta»,17,21-trihydroxy-6«alpha»-methyl-; Pregna-1,4-diene-3,20-dione, 6«alpha»-methyl-11«beta»-17,21-trihydroxy-; Promacortine; Suprametil; U 7532; Urbason; Urbasone; Urbazone; Wyacort; «DELTA»1-6«alpha»-Methylhydrocortisone.

InChI: InChI=1S/C22H30O5/c1-12-8-14-15-5-7-22(27,18(26)11-23)21(15,3)10-17(25)19(14)20(2)6-4-13(24)9-16(12)20/h4,6,9,12,14-15,17,19,23,25,27H,5,7-8,10-11H2,1-3H3

InChI Key: VHRSUDSXCMQTMA-UHFFFAOYSA-N

Formula: C22H30O5

SMILES: CC1CC2C3CCC(O)(C(=O)CO)C3(C)CC(O)C2C2(C)C=CC(=O)C=C12

Molecular Weight: 374.47

CAS: 83-43-2

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-342.13	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-875.53	kJ/mol	Joback Method
$\Delta_{fus} H°$	35.59	kJ/mol	Joback Method
$\Delta_{vap} H°$	122.66	kJ/mol	Joback Method
$logP_{oct/wat}$	1.80		Crippen Method
P_c	1973.55	kPa	Joback Method
T_{boil}	1134.64	K	Joback Method
T_c	1389.79	K	Joback Method
T_{fus}	761.25	K	Joback Method

Property	Value	Unit	Source
V_c	1.09	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1229.87	J/mol×K	1134.64	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C22H30O5/c1-12-8-14-15-5-7-22(27,18(26)11-23)21(15,3)10-17(25)19(14)20(2)6-4-13(24)9-16(12)20/h4,6,9,12,14-15,17,19,23,25,27H,5,7-8,10-11H2,1-3H3

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).