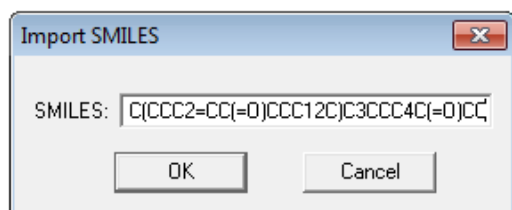
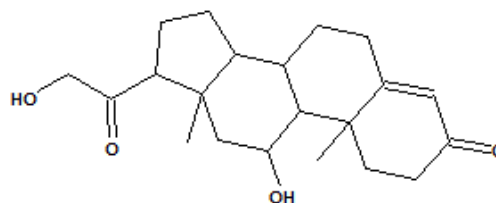
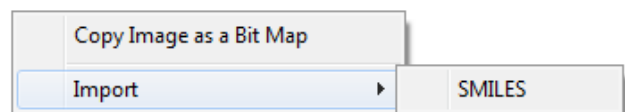


ProPred: Illustration with Corticosterone (CAS Number: 000050-22-6)

Step 1a: Insert the molecular description as SMILES

Or Step 1b: Draw the 2-D molecular structure



Step 2: View the calculated properties (partial list shown)

Summary Marrero and Gani Constantinou and Gani Joback and Reid Wilson Polymers CI_MG Polymers VK

Property Values estimated by using methods included in ProPred

Compound Name : Corticosterone
 Compound CAS : 000050-22-6
 Compound Smiles : OCC(=O)C1CCC2C3CCC4=CC(=O)CCC4(C)C3C(O)CC12C
 Compound Formula : C₂₁H₃₀O₄
 Mw (g/mol) : 346.46

Connectivity Index (CI) values:
 zeroth-order (atomic) CI : 9.67
 first-order (bond) CI : 3.33

PC-Saft parameters:
 m : 11.778100
 sigma : 3.340721
 epsilon : 271.796693

Best estimates are suggested for each property according to developers' criteria. See detailed estimates through each method in the corresponding pages

WARNING:
 Accuracy of some estimated properties (e.g. Hansen parameters) might be poor if the melting point is far above 298 K

Primary Properties

Property	Method	Unit	Est. Value	Exp. Value	Rel. Error	Abs. Error
Tm	MG	K	457.57	454.15	0.75	3.42
Tb	MG	K	701.09	N/A	N/A	N/A
Tc	MG	K	874.41	N/A	N/A	N/A
Pc	MG	bar	17.58	N/A	N/A	N/A
Vc	MG	cm ³ /mol	1050.05	N/A	N/A	N/A
Zc	Wilson		0.220	N/A	N/A	N/A
Gf[298K]	MG	kJ/mol	-395.90	N/A	N/A	N/A
Hf[298K]	MG	kJ/mol	-1163.69	N/A	N/A	N/A
omega	MG		1.716	N/A	N/A	N/A
Hv[298K]	MG	kJ/mol	158.28	N/A	N/A	N/A
Hv[Tb]	MG	kJ/mol	128.93	N/A	N/A	N/A
Hfus	MG	kJ/mol	22.83	N/A	N/A	N/A

Fp	MG	K	679.03	N/A	N/A	N/A
Viscosity	MG	cp	28357.60	N/A	N/A	N/A
THERM.COND	MG	mW/m-K	N/A	N/A	N/A	N/A
<hr/>						
-Log(LC50)FM	MG	Log(mol/L)	3.45	N/A	N/A	N/A
-Log(LC50)DM	*****	Log(mol/L)	N/A	N/A	N/A	N/A
-Log(LD50)	MG	Log(mol/kg)	3.77	N/A	N/A	N/A
Log(BCF)	MG		-0.35	N/A	N/A	N/A
-Log(PEL)	MG	Log(mol/m ³)	6.64	N/A	N/A	N/A
-Log(PCO)	MG		0.30	N/A	N/A	N/A
Log(GWP)	*****		N/A	N/A	N/A	N/A
Log(ODP)	*****		N/A	N/A	N/A	N/A
Log(AP)	*****		N/A	N/A	N/A	N/A
-Log(EUAC)	MG	Log(cas/kg)	5.09	N/A	N/A	N/A
-Log(EUANonC)	*****	Log(cas/kg)	N/A	N/A	N/A	N/A
-Log(ERAC)	MG	Log(cas/kg)	5.26	N/A	N/A	N/A
-Log(ERANonC)	*****	Log(cas/kg)	N/A	N/A	N/A	N/A
-Log(EFWC)	MG	Log(cas/kg)	6.35	N/A	N/A	N/A
-Log(EFWNonC)	*****	Log(cas/kg)	N/A	N/A	N/A	N/A
-Log(ESWC)	MG	Log(cas/kg)	9.32	N/A	N/A	N/A
-Log(ESWNonC)	*****	Log(cas/kg)	N/A	N/A	N/A	N/A
-Log(ENSC)	MG	Log(cas/kg)	7.27	N/A	N/A	N/A
-Log(ENSNonC)	*****	Log(cas/kg)	N/A	N/A	N/A	N/A
-Log(EASC)	MG	Log(cas/kg)	7.05	N/A	N/A	N/A
-Log(EASNonC)	*****	Log(cas/kg)	N/A	N/A	N/A	N/A

Secondary Properties

Property	Method	Unit	Est.Value	Exp.Value	Rel.Error	Abs.Error
Zc	MG		0.254	N/A	N/A	N/A
Sfus	MG	J/(mol*K)	50.26	N/A	N/A	N/A
Vm[Tb]	MG	cm ³ /mol	417.90	N/A	N/A	N/A
Refractive Index	MG		1.27	N/A	N/A	N/A
Molar Refraction	*****		N/A	N/A	N/A	N/A
Closed Flash Temp.	CG	K	534.57	N/A	N/A	N/A
Open Flash Temp.	CG	K	606.27	N/A	N/A	N/A
Dipolar moment	*****	debye	N/A	N/A	N/A	N/A
Dielectric const.	*****		N/A	N/A	N/A	N/A
Henry[298K]	*****	bar*m ³ /mol	N/A	N/A	N/A	N/A
McGowan Volume	Wilson	cm ³ /mol	273.89	N/A	N/A	N/A

MG = Marrero and Gani method
CG = Constantinou and Gani method
JR = Joback and Reid method
Wilson = Wilson method
***** = Method not available

Functional Property (from MG)
Diffusion coefficient at infinite dilution in water

Temp.(K)	Estimated Value (1.0E-5cm ² /s)
464.15	4.458
466.15	4.528
468.15	4.598
470.15	4.669
472.15	4.741
474.15	4.813
476.15	4.887
478.15	4.961
480.15	5.036
482.15	5.112
484.15	5.188

Functional Property (from MG)
Liquid Density

Temp.(K)	Estimated Value (g/cm ³)
464.15	1.8091
466.15	1.8056
468.15	1.8022
470.15	1.7987
472.15	1.7952
474.15	1.7918
476.15	1.7883
478.15	1.7848
480.15	1.7813
482.15	1.7778
484.15	1.7743