

Budesonide

Other names:	(11-«beta»,16-«alpha»)-16,17-(Butylidenebis(oxy))-11,21-dihydroxypregna-1,4-diene-3,20-dione (11-Â«betaÂ»,16-Â«alphaÂ»)-16,17-(Butylidenebis(oxy))-11,21-dihydroxypregna-1,4-diene-3,20-dione (RS)-11«beta»,16«alpha»,17,21-Tetrahydroxypregna-1,4-diene-3,20-dione cyclic 16,17-acetal with butyraldehyde (RS)-11Â«betaÂ»,16Â«alphaÂ»,17,21-Tetrahydroxypregna-1,4-diene-3,20-dione cyclic 16,17-acetal with butyraldehyde 16-«alpha»,17-«alpha»-Butylidenedioxy-11-«beta»,21-dihydroxy-1,4-pregnadiene-3,20-dione 16-Â«alphaÂ»,17-Â«alphaÂ»-Butylidenedioxy-11-Â«betaÂ»,21-dihydroxy-1,4-pregnadiene-3,20-dione (budesonide) 16Â«alphaÂ»,17Â«alphaÂ»-(butylidenedioxy)-11Â«betaÂ»,21-dihydroxypregna-1,4-diene-3,20-dione (budesonide) Budeson Cortivent Entocort Micronyl Preferid Pregna-1,4-diene-3,20-dione, 16,17-[butylidenebis(oxy)]-11,21-dihydroxy-, (11«beta»,16«alpha»)- Pregna-1,4-diene-3,20-dione, 16,17-[butylidenebis(oxy)]-11,21-dihydroxy-, (11Â«betaÂ»,16Â«alphaÂ»)- Pulmicort Respules Rhinocort S-1320 Spirocort
Inchi:	InChI=1S/C25H34O6/c1-4-5-21-30-20-11-17-16-7-6-14-10-15(27)8-9-23(14,2)22(16)18(2)19
InchiKey:	VOVIALXJUBGFJZ-UHFFFAOYSA-N
Formula:	C25H34O6
SMILES:	CCCC1OC2CC3C4CCC5=CC(=O)C=CC5(C)C4C(O)CC3(C)C2(C(=O)CO)O1
Mol. weight [g/mol]:	430.53
CAS:	51333-22-3

Physical Properties

Property code	Value	Unit	Source
gf	-291.54	kJ/mol	Joback Method
hf	-976.42	kJ/mol	Joback Method
hfus	53.37	kJ/mol	Joback Method
hvap	121.60	kJ/mol	Joback Method
log10ws	-4.19		Aqueous Solubility Prediction Method
logp	2.717		Crippen Method

mcvol	326.830	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
tb	1171.74	K	Joback Method
tc	1434.96	K	Joback Method
tf	805.32	K	Joback Method
vc	1.236	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1436.25	J/mol×K	1171.74	Joback Method
cpg	1490.32	J/mol×K	1215.61	Joback Method
cpg	1549.79	J/mol×K	1259.48	Joback Method
cpg	1615.30	J/mol×K	1303.35	Joback Method
cpg	1687.51	J/mol×K	1347.22	Joback Method
cpg	1767.05	J/mol×K	1391.09	Joback Method
cpg	1854.58	J/mol×K	1434.96	Joback Method
hfust	34.70	kJ/mol	534.00	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51333223&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Budesonide, Hydrocortisone, and Prednisolone in Ethanol + Water Mixtures at 298.2 K:	https://www.doi.org/10.1021/je900376r

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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