

hydrocortisone tebutate

Inchi:	InChI=1S/C27H40O6/c1-24(2,3)14-22(31)33-15-21(30)27(32)11-9-19-18-7-6-16-12-17(2)
InchiKey:	FNFPHNZQOKBKHN-UHFFFAOYSA-N
Formula:	C27H40O6
SMILES:	CC(C)(C)CC(=O)OCC(=O)C1(O)CCC2C3CCC4=CC(=O)CCC4(C)C3C(O)CC21C
Mol. weight [g/mol]:	460.61

Physical Properties

Property code	Value	Unit	Source
gf	-416.54	kJ/mol	Joback Method
hf	-1117.49	kJ/mol	Joback Method
hfus	37.54	kJ/mol	Joback Method
hvap	124.99	kJ/mol	Joback Method
log10ws	-5.51		Aqueous Solubility Prediction Method
logp	3.769		Crippen Method
mcvol	365.870	ml/mol	McGowan Method
pc	1311.80	kPa	Joback Method
tb	1235.43	K	Joback Method
tc	1518.30	K	Joback Method
tf	834.84	K	Joback Method
vc	1.377	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1635.64	J/mol×K	1235.43	Joback Method
cpg	1701.29	J/mol×K	1282.58	Joback Method
cpg	1773.76	J/mol×K	1329.72	Joback Method
cpg	1853.82	J/mol×K	1376.87	Joback Method
cpg	1942.26	J/mol×K	1424.01	Joback Method
cpg	2039.88	J/mol×K	1471.16	Joback Method
cpg	2147.46	J/mol×K	1518.30	Joback Method

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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