

prednisolone-21-trimethylacetate

Inchi: InChI=1S/C26H36O6/c1-23(2,3)22(30)32-14-20(29)26(31)11-9-18-17-7-6-15-12-16(27)8
InchiKey: PHEOVVDXTQVHAZ-UHFFFAOYSA-N
Formula: C₂₆H₃₆O₆
SMILES: CC(C)(C)C(=O)OCC(=O)C1(O)CCC2C3CCC4=CC(=O)C=CC4(C)C3C(O)CC21C
Mol. weight [g/mol]: 444.57

Physical Properties

Property code	Value	Unit	Source
gf	-395.00	kJ/mol	Joback Method
hf	-1039.07	kJ/mol	Joback Method
hfus	36.17	kJ/mol	Joback Method
hvap	123.06	kJ/mol	Joback Method
log10ws	-4.58		Aqueous Solubility Prediction Method
logp	3.155		Crippen Method
mcvol	347.480	ml/mol	McGowan Method
pc	1446.83	kPa	Joback Method
tb	1211.71	K	Joback Method
tc	1485.49	K	Joback Method
tf	824.33	K	Joback Method
vc	1.306	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1515.50	J/molxK	1211.71	Joback Method
cpg	1574.99	J/molxK	1257.34	Joback Method
cpg	1640.62	J/molxK	1302.97	Joback Method
cpg	1713.10	J/molxK	1348.60	Joback Method
cpg	1793.14	J/molxK	1394.23	Joback Method
cpg	1881.46	J/molxK	1439.86	Joback Method
cpg	1978.75	J/molxK	1485.49	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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

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

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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