11Beta,17alpha-dihydroxy-2alpha,21-diacetoxypre

Inchi: InChI=1S/C25H34O8/c1-13(26)32-12-21(30)25(31)8-7-17-16-6-5-15-9-18(28)20(33-14(2)
InchiKey: OSXMUKKFZOIHEW-CQCMRUBDSA-N
Formula: C25H34O8
SMILES: CC(=O)OCC(=O)C1(O)CCC2C3CCC4=CC(=O)C(OC(C)=O)CC4(C)C3C(O)CC21C
Mol. weight [g/mol]: 462.53

Physical Properties

Property code	Value	Unit	Source
gf	-677.85	kJ/mol	Joback Method
hf	-1332.60	kJ/mol	Joback Method
hfus	43.63	kJ/mol	Joback Method
hvap	130.68	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	1.894		Crippen Method
mcvol	345.130	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
tb	1264.52	K	Joback Method
tc	1558.32	K	Joback Method
tf	877.80	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1557.33	J/mol×K	1264.52	Joback Method
cpg	1621.67	J/mol×K	1313.49	Joback Method
cpg	1692.59	J/mol×K	1362.45	Joback Method
cpg	1770.85	J/mol×K	1411.42	Joback Method
cpg	1857.19	J/mol×K	1460.39	Joback Method
cpg	1952.38	J/mol×K	1509.35	Joback Method
cpg	2057.16	J/mol×K	1558.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005436&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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