4-Pregnene-3,11,20-trione, 17alpha,21-dihydroxy-, 21-acetate

Other names: 17Alpha,21 dihydroxypregna-4-ene-3,11,20-trione,21 acetate
Inchi: InChI=1S/C23H30O6/c1-13(24)29-12-19(27)23(28)9-7-17-16-5-4-14-10-15(25)6-8-21(14
InchiKey: ITRJWOMZKQRYTA-UHFFFAOYSA-N
Formula: C23H30O6
SMILES: CC(=O)OCC(=O)C1(O)CCC2C3CCC4=CC(=O)CCC4(C)C3C(=O)CC21C
Mol. weight [g/mol]: 402.48
CAS: 96843-92-4

Physical Properties

Property code	Value	Unit	Source
gf	-431.12	kJ/mol	Joback Method
hf	-991.31	kJ/mol	Joback Method
hfus	28.94	kJ/mol	Joback Method
hvap	105.26	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.561		Crippen Method
mcvol	305.210	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
tb	1127.45	K	Joback Method
tc	1385.62	K	Joback Method
tf	798.98	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1258.01	J/mol×K	1127.45	Joback Method
cpg	1300.55	J/mol×K	1170.48	Joback Method
cpg	1346.67	J/mol×K	1213.51	Joback Method
cpg	1396.87	J/mol×K	1256.53	Joback Method
cpg	1451.65	J/mol×K	1299.56	Joback Method
cpg	1511.50	J/mol×K	1342.59	Joback Method
cpg	1576.91	J/mol×K	1385.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96843924&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
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