17Alpha-acetoxy-6alpha-methyl-pregn-4-ene-3,20-

Inchi: InChI=1S/C24H34O4/c1-14-12-18-19(22(4)9-6-17(27)13-21(14)22)7-10-23(5)20(18)8-11-24(23)28-16(3)26)15(2)25/h12-13,15,18-20H,6-11H2,1-5H3/t15-,18+,19-,20-,22+,23-,24-/m0/s1

InchiKey: PSGAAPLEWMOORI-JTOXMAKQSA-N

Formula: C24H34O4

SMILES: CC(=O)OC1(C(C)=O)CCC2C3CC(C)C4=CC(=O)CCC4(C)C3CCC21C

Mol. weight [g/mol]: 386.52

CAS: 560-12-3

Physical Properties

Property code	Value	Unit	Source
gf	-171.00	kJ/mol	Joback Method
hf	-742.36	kJ/mol	Joback Method
hfus	29.00	kJ/mol	Joback Method
hvap	86.25	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.655		Crippen Method
mcvol	311.860	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
tb	985.66	K	Joback Method
tc	1235.06	K	Joback Method
tf	676.97	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.88	J/mol×K	985.66	Joback Method
cpg	1211.56	J/mol×K	1027.23	Joback Method
cpg	1248.23	J/mol×K	1068.79	Joback Method
cpg	1287.38	J/mol×K	1110.36	Joback Method
cpg	1329.49	J/mol×K	1151.93	Joback Method
cpg	1375.04	J/mol×K	1193.50	Joback Method
cpg	1424.53	J/mol×K	1235.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C560123&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