5Beta-androstan-12-one,17beta-acetamido-3alpha

Inchi: InChI=1S/C23H35NO4/c1-13(25)24-20-8-7-18-17-6-5-15-11-16(28-14(2)26)9-10-22(15,3
InchiKey: JLPROZIQMZUUDI-UHFFFAOYSA-N
Formula: C23H35NO4
SMILES: CC(=O)NC1CCC2C3CCC4CC(OC(C)=O)CCC4(C)C3CC(=O)C12C
Mol. weight [g/mol]: 389.53
CAS: 16319-63-4

Physical Properties

Property code	Value	Unit	Source
gf	-112.58	kJ/mol	Joback Method
hf	-750.14	kJ/mol	Joback Method
hfus	38.05	kJ/mol	Joback Method
hvap	90.35	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.645		Crippen Method
mcvol	312.050	ml/mol	McGowan Method
pc	1406.95	kPa	Joback Method
tb	1003.90	K	Joback Method
tc	1248.86	K	Joback Method
tf	676.94	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1210.40	J/mol×K	1003.90	Joback Method
cpg	1239.74	J/mol×K	1044.73	Joback Method
cpg	1269.71	J/mol×K	1085.55	Joback Method
cpg	1300.63	J/mol×K	1126.38	Joback Method
cpg	1332.85	J/mol×K	1167.20	Joback Method
cpg	1366.70	J/mol×K	1208.03	Joback Method
cpg	1402.51	J/mol×K	1248.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16319634&Units=SI

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