5Alpha-pregnan-20-one, 16alpha, 17alpha-epoxy-3beta-hydroxy-, acetate

Inchi: InChI=1S/C23H34O4/c1-13(24)23-20(27-23)12-19-17-6-5-15-11-16(26-14(2)25)7-9-21(1

InchiKey: BDJNJWJAJKMWQI-UHFFFAOYSA-N

Formula: C23H34O4

SMILES: CC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C3CC3OC32C(C)=O)C1

Mol. weight [g/mol]: 374.51

CAS: 2066-51-5

Physical Properties

Property code	Value	Unit	Source
gf	-86.04	kJ/mol	Joback Method
hf	-697.55	kJ/mol	Joback Method
hfus	37.46	kJ/mol	Joback Method
hvap	82.60	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.297		Crippen Method
mcvol	295.510	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
tb	911.30	K	Joback Method
tc	1150.72	K	Joback Method
tf	631.51	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1102.69	J/mol×K	911.30	Joback Method
cpg	1134.05	J/mol×K	951.20	Joback Method
cpg	1167.01	J/mol×K	991.11	Joback Method
cpg	1202.10	J/mol×K	1031.01	Joback Method
cpg	1239.83	J/mol×K	1070.92	Joback Method
cpg	1280.73	J/mol×K	1110.82	Joback Method
cpg	1325.32	J/mol×K	1150.72	Joback Method

Sources

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=C2066515&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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