24-Nor-5,22-cholestadienol (E) acetate

Inchi: InChI=1S/C26H40O2/c1-6-7-17(2)22-10-11-23-21-9-8-19-16-20(28-18(3)27)12-14-25(19
InchiKey: JIBKZRVQNXWAED-SBFOJMOBSA-N
Formula: C26H40O2
SMILES: CC=CC(C)C1CCC2C3CC=C4CC(OC(C)=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	180.62	kJ/mol	Joback Method
hf	-436.66	kJ/mol	Joback Method
hfus	36.05	kJ/mol	Joback Method
hvap	80.43	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	6.709		Crippen Method
mcvol	332.600	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rinpol	3026.00		NIST Webbook
tb	913.21	K	Joback Method
tc	1146.78	K	Joback Method
tf	537.38	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1199.77	J/mol×K	913.21	Joback Method
cpg	1229.42	J/mol×K	952.14	Joback Method
cpg	1259.36	J/mol×K	991.07	Joback Method
cpg	1289.95	J/mol×K	1029.99	Joback Method
cpg	1321.56	J/mol×K	1068.92	Joback Method
cpg	1354.55	J/mol×K	1107.85	Joback Method
cpg	1389.27	J/mol×K	1146.78	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=R489880&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume