Cholestanol acetate

Other names: Coprostanol acetate
Inchi: InChI=1S/C29H50O2/c1-19(2)8-7-9-20(3)25-12-13-26-24-11-10-22-18-23(31-21(4)30)14
InchiKey: PHLIUSDPFOUISN-FJHKFUNJSA-N
Formula: C29H50O2
SMILES: CC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]: 430.71
CAS: 4947-63-1

Physical Properties

Property code	Value	Unit	Source
gf	95.18	kJ/mol	Joback Method
hf	-687.73	kJ/mol	Joback Method
hfus	40.34	kJ/mol	Joback Method
hvap	85.50	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	8.039		Crippen Method
mcvol	383.470	ml/mol	McGowan Method
pc	898.02	kPa	Joback Method
rinpol	3193.00		NIST Webbook
rinpol	3125.00		NIST Webbook
tb	968.44	K	Joback Method
tc	1195.48	K	Joback Method
tf	543.75	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1465.89	J/mol×K	968.44	Joback Method
cpg	1498.65	J/mol×K	1006.28	Joback Method
cpg	1531.69	J/mol×K	1044.12	Joback Method
cpg	1565.33	J/mol×K	1081.96	Joback Method
cpg	1599.90	J/mol×K	1119.80	Joback Method
cpg	1635.71	J/mol×K	1157.64	Joback Method

cpg	1673.10	J/mol×K	1195.48	Joback Method

Sources

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=C4947631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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