24-Ethyl-22-coprostenol acetate

Inchi: InChI=1S/C31H52O2/c1-8-23(20(2)3)10-9-21(4)27-13-14-28-26-12-11-24-19-25(33-22(5)
InchiKey: SNLRWRYYFMQYJK-WTNZWOCRSA-N
Formula: C31H52O2
SMILES: CCC(C=CC(C)C1CCC2C3CCC4CC(OC(C)=O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 456.74

Physical Properties

Property code	Value	Unit	Source
gf	189.80	kJ/mol	Joback Method
hf	-617.07	kJ/mol	Joback Method
hfus	42.19	kJ/mol	Joback Method
hvap	89.52	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	8.451		Crippen Method
mcvol	407.350	ml/mol	McGowan Method
pc	830.98	kPa	Joback Method
rinpol	3253.00		NIST Webbook
tb	1017.92	K	Joback Method
tc	1252.40	K	Joback Method
tf	546.21	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1582.57	J/mol×K	1017.92	Joback Method
cpg	1618.34	J/mol×K	1057.00	Joback Method
cpg	1654.95	J/mol×K	1096.08	Joback Method
cpg	1692.80	J/mol×K	1135.16	Joback Method
cpg	1732.25	J/mol×K	1174.24	Joback Method
cpg	1773.70	J/mol×K	1213.32	Joback Method
cpg	1817.52	J/mol×K	1252.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110282&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume