28-Isoavenasterol acetate

Inchi: InChI=1S/C32H52O2/c1-9-24(21(2)3)11-10-22(4)27-15-18-32(8)29-13-12-25-20-26(34-2
InchiKey: UKBUAVLRSUYDBZ-FABCEXJGSA-N
Formula: C32H52O2
SMILES: CC=C(CCC(C)C1CCC2(C)C3=CCC4CC(OC(C)=O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	214.66	kJ/mol	Joback Method
hf	-560.33	kJ/mol	Joback Method
hfus	40.46	kJ/mol	Joback Method
hvap	92.33	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.906		Crippen Method
mcvol	417.140	ml/mol	McGowan Method
pc	830.98	kPa	Joback Method
rinpol	3406.00		NIST Webbook
rinpol	3406.00		NIST Webbook
tb	1050.17	K	Joback Method
tc	1290.62	K	Joback Method
tf	599.94	K	Joback Method
vc	1.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1636.59	J/mol×K	1050.17	Joback Method
cpg	1681.51	J/mol×K	1090.25	Joback Method
cpg	1729.22	J/mol×K	1130.32	Joback Method
cpg	1780.25	J/mol×K	1170.40	Joback Method
cpg	1835.14	J/mol×K	1210.47	Joback Method
cpg	1894.42	J/mol×K	1250.55	Joback Method
cpg	1958.64	J/mol×K	1290.62	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=R110599&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