Agnosterol acetate

Inchi: InChI=1S/C32H50O2/c1-21(2)11-10-12-22(3)24-15-19-32(9)26-13-14-27-29(5,6)28(34-23
InchiKey: SJXLZCIHOACHCY-XKRINNQWSA-N
Formula: C32H50O2
SMILES: CC(=O)OC1CCC2(C)C3=CCC4(C)C(C(C)CCC=C(C)C)CCC4(C)C3=CCC2C1(C)C
Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	231.94	kJ/mol	Joback Method
hf	-493.50	kJ/mol	Joback Method
hfus	38.52	kJ/mol	Joback Method
hvap	92.52	kJ/mol	Joback Method
log10ws	-9.64		Crippen Method
logp	8.826		Crippen Method
mcvol	412.840	ml/mol	McGowan Method
pc	859.48	kPa	Joback Method
rinpol	3316.00		NIST Webbook
rinpol	3316.00		NIST Webbook
tb	1054.99	K	Joback Method
tc	1298.03	K	Joback Method
tf	652.12	K	Joback Method
vc	1.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1621.27	J/mol×K	1054.99	Joback Method
cpg	1673.78	J/mol×K	1095.50	Joback Method
cpg	1730.72	J/mol×K	1136.00	Joback Method
cpg	1792.76	J/mol×K	1176.51	Joback Method
cpg	1860.58	J/mol×K	1217.02	Joback Method
cpg	1934.83	J/mol×K	1257.52	Joback Method
cpg	2016.17	J/mol×K	1298.03	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=R489939&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