24-Dehydropollinastanol acetate

Inchi: InChI=1S/C29H46O2/c1-19(2)7-8-20(3)24-12-13-27(6)25-10-9-22-17-23(31-21(4)30)11-1
InchiKey: KCDCVYFVHAXYGG-LEQFWYBKSA-N
Formula: C29H46O2
SMILES: CC(=O)OC1CCC23CC24CCC2(C)C(C(C)CC=C(C)C)CCC2(C)C4CCC3C1
Mol. weight [g/mol]: 426.67

Physical Properties

Property code	Value	Unit	Source
gf	250.97	kJ/mol	Joback Method
hf	-439.08	kJ/mol	Joback Method
hfus	31.42	kJ/mol	Joback Method
hvap	83.50	kJ/mol	Joback Method
log10ws	-8.33		Crippen Method
logp	7.713		Crippen Method
mcvol	368.310	ml/mol	McGowan Method
pc	1050.73	kPa	Joback Method
rinpol	3272.00		NIST Webbook
tb	976.27	K	Joback Method
tc	1215.81	K	Joback Method
tf	616.73	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1419.81	J/mol×K	976.27	Joback Method
cpg	1464.53	J/mol×K	1016.19	Joback Method
cpg	1512.92	J/mol×K	1056.12	Joback Method
cpg	1565.67	J/mol×K	1096.04	Joback Method
cpg	1623.47	J/mol×K	1135.97	Joback Method
cpg	1687.04	J/mol×K	1175.89	Joback Method
cpg	1757.07	J/mol×K	1215.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110193&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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