Pollinastanol acetate

Inchi: InChI=1S/C29H48O2/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: XWQUCCSOTWFBSU-LEQFWYBKSA-N
Formula: C29H48O2
SMILES: CC(=O)OC1CCC23CC24CCC2(C)C(C(C)CCC(C)C)CCC2(C)C4CCC3C1
Mol. weight [g/mol]: 428.69

Physical Properties

Property code	Value	Unit	Source
gf	176.86	kJ/mol	Joback Method
hf	-551.79	kJ/mol	Joback Method
hfus	29.00	kJ/mol	Joback Method
hvap	83.08	kJ/mol	Joback Method
log10ws	-8.23		Crippen Method
logp	7.793		Crippen Method
mcvol	372.610	ml/mol	McGowan Method
pc	1018.13	kPa	Joback Method
rinpol	3240.00		NIST Webbook
tb	971.79	K	Joback Method
tc	1206.62	K	Joback Method
tf	620.77	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1446.25	J/mol×K	971.79	Joback Method
cpg	1489.85	J/mol×K	1010.93	Joback Method
cpg	1536.68	J/mol×K	1050.07	Joback Method
cpg	1587.37	J/mol×K	1089.21	Joback Method
cpg	1642.56	J/mol×K	1128.35	Joback Method
cpg	1702.90	J/mol×K	1167.49	Joback Method
cpg	1769.03	J/mol×K	1206.62	Joback Method

Sources

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=R111403&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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