Lanost-9(11)-en-3-ol, acetate, (3«beta»,8«alpha»,13«alpha»,14«beta»,17«alpha»)

Other names: parkeol acetylated
Inchi: InChI=1S/C32H54O2/c1-21(2)11-10-12-22(3)24-15-19-32(9)26-13-14-27-29(5,6)28(34-2
InchiKey: BUEBATVTSJOJKD-NCKBGQQQSA-N
Formula: C32H54O2
SMILES: CC(=O)OC1CCC2(C)C3=CCC4(C)C(C(C)CCCC(C)C)CCC4(C)C3CCC2C1(C)C
Mol. weight [g/mol]: 470.77
CAS: 55515-26-9

Physical Properties

Property code	Value	Unit	Source
gf	129.79	kJ/mol	Joback Method
hf	-672.86	kJ/mol	Joback Method
hfus	36.34	kJ/mol	Joback Method
hvap	90.83	kJ/mol	Joback Method
log10ws	-9.45		Crippen Method
logp	8.986		Crippen Method
mcvol	421.440	ml/mol	McGowan Method
pc	809.83	kPa	Joback Method
rinpol	3296.00		NIST Webbook
rinpol	3296.00		NIST Webbook
tb	1041.70	K	Joback Method
tc	1279.77	K	Joback Method
tf	638.64	K	Joback Method
vc	1.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1677.94	J/mol×K	1041.70	Joback Method
cpg	1728.28	J/mol×K	1081.38	Joback Method
cpg	1782.26	J/mol×K	1121.06	Joback Method
cpg	1840.47	J/mol×K	1160.73	Joback Method
cpg	1903.53	J/mol×K	1200.41	Joback Method
cpg	1972.04	J/mol×K	1240.09	Joback Method

cpg	2046.59	J/mol×K	1279.77	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55515269&Units=SI

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