31-Norcyclolaudenol acetate

Inchi: InChI=1S/C32H52O2/c1-20(2)21(3)9-10-22(4)24-11-12-25-26-13-14-27-29(6,7)28(34-23
InchiKey: QIUMNCOQNZKHEF-MNTLUMBWSA-N
Formula: C32H52O2
SMILES: C=C(C)C(C)CCC(C)C1CCC2C3CCC4C(C)(C)C(OC(C)=O)CCC45CC35CCC12C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	273.70	kJ/mol	Joback Method
hf	-518.41	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	88.86	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.596		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	861.00	kPa	Joback Method
rinpol	3367.00		NIST Webbook
rinpol	3367.00		NIST Webbook
tb	1032.32	K	Joback Method
tc	1270.96	K	Joback Method
tf	634.62	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1649.30	J/mol×K	1032.32	Joback Method
cpg	1700.86	J/mol×K	1072.09	Joback Method
cpg	1756.63	J/mol×K	1111.87	Joback Method
cpg	1817.30	J/mol×K	1151.64	Joback Method
cpg	1883.55	J/mol×K	1191.41	Joback Method
cpg	1956.06	J/mol×K	1231.19	Joback Method
cpg	2035.52	J/mol×K	1270.96	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=R110673&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