

9,19-Cyclolanostan-3-ol, 24-methylene-, acetate, (3«beta»)-

Other names:	24-methylene-cycloartenol, acetylated
Inchi:	InChI=1S/C33H54O2/c1-21(2)22(3)10-11-23(4)25-14-16-31(9)27-13-12-26-29(6,7)28(35)
InchiKey:	BYIMYSSYXBYIBJ-UHFFFAOYSA-N
Formula:	C33H54O2
SMILES:	C=C(CCC(C)C1CCC2(C)C3CCC4C(C)(C)C(OC(C)=O)CCC45CC35CCC12C)C(C)C
Mol. weight [g/mol]:	482.78
CAS:	1259-94-5

Physical Properties

Property code	Value	Unit	Source
gf	276.63	kJ/mol	Joback Method
hf	-523.81	kJ/mol	Joback Method
hfus	31.55	kJ/mol	Joback Method
hvap	89.93	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	8.986		Crippen Method
mcvol	424.670	ml/mol	McGowan Method
pc	835.79	kPa	Joback Method
rinpol	3365.00		NIST Webbook
rinpol	3365.00		NIST Webbook
tb	1055.44	K	Joback Method
tc	1298.17	K	Joback Method
tf	669.79	K	Joback Method
vc	1.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1746.73	J/molxK	1055.44	Joback Method
cpg	1809.70	J/molxK	1095.89	Joback Method
cpg	1878.87	J/molxK	1136.35	Joback Method
cpg	1955.08	J/molxK	1176.80	Joback Method
cpg	2039.17	J/molxK	1217.26	Joback Method
cpg	2131.98	J/molxK	1257.71	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=C1259945&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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