24-Methyllanostanol acetate

Inchi: InChI=1S/C33H58O2/c1-21(2)22(3)11-12-23(4)25-15-19-33(10)27-13-14-28-30(6,7)29(3
InchiKey: YFYYDOQQCHZXIX-JZFRLXDESA-N
Formula: C33H58O2
SMILES: CC(=O)OC1CCC2(C)C3CCC4(C)C(C(C)CCC(C)C(C)C)CCC4(C)C3CCC2C1(C)C
Mol. weight [g/mol]: 486.81

Physical Properties

Property code	Value	Unit	Source
gf	107.73	kJ/mol	Joback Method
hf	-765.43	kJ/mol	Joback Method
hfus	35.65	kJ/mol	Joback Method
hvap	91.41	kJ/mol	Joback Method
log10ws	-9.53		Crippen Method
logp	9.312		Crippen Method
mcvol	439.830	ml/mol	McGowan Method
pc	748.15	kPa	Joback Method
rinpol	3485.00		NIST Webbook
rinpol	3485.00		NIST Webbook
tb	1055.33	K	Joback Method
tc	1294.80	K	Joback Method
tf	617.39	K	Joback Method
vc	1.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1789.86	J/mol×K	1055.33	Joback Method
cpg	1842.78	J/mol×K	1095.24	Joback Method
cpg	1899.38	J/mol×K	1135.15	Joback Method
cpg	1960.26	J/mol×K	1175.07	Joback Method
cpg	2026.04	J/mol×K	1214.98	Joback Method
cpg	2097.35	J/mol×K	1254.89	Joback Method
cpg	2174.79	J/mol×K	1294.80	Joback Method

Sources

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=R110544&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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