

Lanostan-3-yl acetate

Other names:	CI4502
	Lanostanol acetate
Inchi:	InChI=1S/C32H56O2/c1-21(2)11-10-12-22(3)24-15-19-32(9)26-13-14-27-29(5,6)28(34-2
InchiKey:	GBJJVPUZVRPWOZ-UHFFFAOYSA-N
Formula:	C32H56O2
SMILES:	CC(=O)OC1CCC2(C)C3CCC4(C)C(C(C)CCCC(C)C)CCC4(C)C3CCC2C1(C)C
Mol. weight [g/mol]:	472.79

Physical Properties

Property code	Value	Unit	Source
gf	101.75	kJ/mol	Joback Method
hf	-739.51	kJ/mol	Joback Method
hfus	36.58	kJ/mol	Joback Method
hvap	89.57	kJ/mol	Joback Method
log10ws	-9.35		Crippen Method
logp	9.066		Crippen Method
mcvol	425.740	ml/mol	McGowan Method
pc	785.51	kPa	Joback Method
rinpol	3393.00		NIST Webbook
rinpol	3393.00		NIST Webbook
tb	1032.89	K	Joback Method
tc	1268.99	K	Joback Method
tf	621.12	K	Joback Method
vc	1.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1708.73	J/mol×K	1032.89	Joback Method
cpg	1758.43	J/mol×K	1072.24	Joback Method
cpg	1811.41	J/mol×K	1111.59	Joback Method
cpg	1868.27	J/mol×K	1150.94	Joback Method
cpg	1929.59	J/mol×K	1190.29	Joback Method
cpg	1995.96	J/mol×K	1229.64	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=U332396&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

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