

31-Norlanosterol acetate

Inchi: InChI=1S/C31H50O2/c1-9-10-11-12-21(2)23-15-19-31(8)25-13-14-26-28(4,5)27(33-22(3)24)30-29-31
InchiKey: QBLZWFPDPZVSOO-JHBUWWQPSA-N
Formula: C31H50O2
SMILES: CC=CCCC(C)C1CCC2(C)C3=C(CCC12C)C1(C)CCC(OC(C)=O)C(C)(C)C1CC3
Mol. weight [g/mol]: 454.73

Physical Properties

Property code	Value	Unit	Source
gf	202.11	kJ/mol	Joback Method
hf	-520.85	kJ/mol	Joback Method
hfus	36.02	kJ/mol	Joback Method
hvap	89.92	kJ/mol	Joback Method
log10ws	-9.37		Crippen Method
logp	8.660		Crippen Method
mcvol	403.050	ml/mol	McGowan Method
pc	887.88	kPa	Joback Method
rinpol	3278.00		NIST Webbook
rinpol	3278.00		NIST Webbook
tb	1033.07	K	Joback Method
tc	1273.05	K	Joback Method
tf	654.05	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1574.29	J/mol×K	1033.07	Joback Method
cpg	1623.78	J/mol×K	1073.07	Joback Method
cpg	1677.19	J/mol×K	1113.06	Joback Method
cpg	1735.16	J/mol×K	1153.06	Joback Method
cpg	1798.32	J/mol×K	1193.06	Joback Method
cpg	1867.31	J/mol×K	1233.05	Joback Method
cpg	1942.75	J/mol×K	1273.05	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=R110688&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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