Clionasterol acetate

Inchi:	InChI=1S/C31H52O2/c1-8-23(20(2)3)10-9-21(4)27-13-14-28-26-12-11-24-19-25(33-22(5
InchiKey:	PBWOIPCULUXTNY-ZWFWBUGJSA-N
Formula:	C31H52O2
SMILES:	CCC(CCC(C)C1CCC2C3CC=C4CC(OC(C)=O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]:	456.74
CAS:	4651-54-1

Physical Properties

Property code	Value	Unit	Source
gf	137.62	kJ/mol	Joback Method
hf	-667.64	kJ/mol	Joback Method
hfus	41.75	kJ/mol	Joback Method
hvap	90.83	kJ/mol	Joback Method
log10ws	-9.03		Crippen Method
logp	8.596		Crippen Method
mcvol	407.350	ml/mol	McGowan Method
pc	831.94	kPa	Joback Method
rinpol	3355.00		NIST Webbook
tb	1022.57	K	Joback Method
tc	1255.94	K	Joback Method
tf	568.81	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1576.09	J/mol×K	1022.57	Joback Method
cpg	1611.24	J/mol×K	1061.47	Joback Method
cpg	1647.21	J/mol×K	1100.36	Joback Method
cpg	1684.37	J/mol×K	1139.26	Joback Method
cpg	1723.09	J/mol×K	1178.15	Joback Method
cpg	1763.71	J/mol×K	1217.05	Joback Method
cpg	1806.62	J/mol×K	1255.94	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=C4651541&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

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