

Cholest-5-en-3-ol (3«beta»)-, nonanoate

Other names:	Cholesterol, nonanoate Cholesterol pelargonate Cholesteryl nonanoate Cholesteryl nonylate Cholesteryl pelargonate 5-Cholesten-3«beta»-ol pelargonate cholest-5-ene-3-beta-yl nonanoate
Inchi:	InChI=1S/C36H62O2/c1-7-8-9-10-11-12-16-34(37)38-29-21-23-35(5)28(25-29)17-18-30-
InchiKey:	WCLNGBQPTVENHV-SPICIWKBSA-N
Formula:	C36H62O2
SMILES:	<chem>CCCCCCCCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1</chem>
Mol. weight [g/mol]:	526.88
CAS:	1182-66-7

Physical Properties

Property code	Value	Unit	Source
gf	182.16	kJ/mol	Joback Method
hf	-765.56	kJ/mol	Joback Method
hfus	58.23	kJ/mol	Joback Method
hvap	102.35	kJ/mol	Joback Method
log10ws	-11.37		Crippen Method
logp	10.690		Crippen Method
mcvol	477.800	ml/mol	McGowan Method
pc	639.30	kPa	Joback Method
tb	1137.41	K	Joback Method
tc	1396.89	K	Joback Method
tf	640.16	K	Joback Method
vc	1.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1953.79	J/molxK	1137.41	Joback Method
cpg	2000.65	J/molxK	1180.66	Joback Method

cpg	2049.70	J/mol×K	1223.90	Joback Method
cpg	2101.45	J/mol×K	1267.15	Joback Method
cpg	2156.46	J/mol×K	1310.40	Joback Method
cpg	2215.23	J/mol×K	1353.64	Joback Method
cpg	2278.31	J/mol×K	1396.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1182667&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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