Cholesterol, propyl carbonate

Inchi: InChI=1S/C31H52O3/c1-7-19-33-29(32)34-24-15-17-30(5)23(20-24)11-12-25-27-14-13-2
InchiKey: HDCRAXGDAFODLS-UHFFFAOYSA-N
Formula: C31H52O3
SMILES: CCCOC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]: 472.74
CAS: 38577-26-3

Physical Properties

Property code	Value	Unit	Source
gf	35.06	kJ/mol	Joback Method
hf	-794.58	kJ/mol	Joback Method
hfus	46.46	kJ/mol	Joback Method
hvap	93.63	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.960		Crippen Method
mcvol	413.220	ml/mol	McGowan Method
pc	820.07	kPa	Joback Method
tb	1045.43	K	Joback Method
tc	1281.05	K	Joback Method
tf	606.04	K	Joback Method
vc	1.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1614.36	J/mol×K	1045.43	Joback Method
cpg	1649.88	J/mol×K	1084.70	Joback Method
cpg	1686.27	J/mol×K	1123.97	Joback Method
cpg	1723.88	J/mol×K	1163.24	Joback Method
cpg	1763.06	J/mol×K	1202.51	Joback Method
cpg	1804.18	J/mol×K	1241.78	Joback Method
cpg	1847.58	J/mol×K	1281.05	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=C38577263&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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