Cholesteryl benzoate

Other names:	5-Cholesten-3«beta»-ol benzoate
	Cholesterol benzoate
	Cholest-5-en-3-ol (3«beta»)-, benzoate
	cholest-5-ene-3-beta-yl benzoate
Inchi:	InChI=1S/C34H50O2/c1-23(2)10-9-11-24(3)29-16-17-30-28-15-14-26-22-27(36-32(35)25
InchiKey:	UVZUFUGNHDDLRQ-QGRFRJTBSA-N
Formula:	C34H50O2
SMILES:	CC(C)CCCC(C)C1CCC2C3CC=C4CC(OC(=O)c5ccccc5)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	490.76
CAS:	604-32-0

Physical Properties

Property code	Value	Unit	Source
gf	277.73	kJ/mol	Joback Method
hf	-487.75	kJ/mol	Joback Method
hfus	47.09	kJ/mol	Joback Method
hvap	100.17	kJ/mol	Joback Method
log10ws	-10.21		Crippen Method
logp	9.253		Crippen Method
mcvol	425.860	ml/mol	McGowan Method
pc	849.00	kPa	Joback Method
tb	1118.33	K	Joback Method
tc	1371.90	K	Joback Method
tf	644.04	K	Joback Method
vc	1.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1700.28	J/mol×K	1118.33	Joback Method
cpg	1741.66	J/mol×K	1160.59	Joback Method
cpg	1785.20	J/mol×K	1202.85	Joback Method
cpg	1831.38	J/mol×K	1245.12	Joback Method
cpg	1880.70	J/mol×K	1287.38	Joback Method

cpg	1933.65	J/mol×K	1329.64	Joback Method
cpg	1990.74	J/mol×K	1371.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C604320&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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