

Cholesteryl normal-heptylate

Other names:	Cholesteryl enanthate Cholesteryl heptanoate Cholesteryl heptonate Cholest-5-en-3-ol (3«beta»)-, heptanoate 3«beta»-Heptanoyloxycholest-5-ene cholesteryl n-heptylate cholest-5-ene-3-beta-yl heptanoate
Inchi:	InChI=1S/C34H58O2/c1-7-8-9-10-14-32(35)36-27-19-21-33(5)26(23-27)15-16-28-30-18-
InchiKey:	KXWDMNPRHKRGKB-JKZRPSLESA-N
Formula:	C34H58O2
SMILES:	CCCCCCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]:	498.82
CAS:	1182-07-6

Physical Properties

Property code	Value	Unit	Source
gf	165.32	kJ/mol	Joback Method
hf	-724.28	kJ/mol	Joback Method
hfus	53.05	kJ/mol	Joback Method
hvap	97.89	kJ/mol	Joback Method
log10ws	-10.53		Crippen Method
logp	9.910		Crippen Method
mcvol	449.620	ml/mol	McGowan Method
pc	706.21	kPa	Joback Method
tb	1091.65	K	Joback Method
tc	1336.75	K	Joback Method
tf	387.30 ± 0.50	K	NIST Webbook
vc	1.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1799.10	J/mol×K	1091.65	Joback Method
cpg	1840.20	J/mol×K	1132.50	Joback Method

cpg	1882.82	J/mol×K	1173.35	Joback Method
cpg	1927.40	J/mol×K	1214.20	Joback Method
cpg	1974.36	J/mol×K	1255.05	Joback Method
cpg	2024.15	J/mol×K	1295.90	Joback Method
cpg	2077.20	J/mol×K	1336.75	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=C1182076&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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