Cholest-5-en-3-ol (3«beta»)-, 9-octadecenoate, (Z)-

Other names: Cholesterol, oleate
Cholesteroyl-oleate
Cholesteryl cis-9-octadecenoate
Cholesteryl oleate
Oleoylcholesterol
cholest-5-en-3-«beta»-yl oleate

Inchi: InChI=1S/C45H78O2/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-43(46)47-38-30

InchiKey: RJECHNNFRHZQKU-VDPFXVTESA-N

Formula: C45H78O2

SMILES: CCCCCCCCC=CCCCCCCCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCCC(C)C

Mol. weight [g/mol]: 651.10

CAS: 303-43-5

Physical Properties

Property code	Value	Unit	Source
gf	338.16	kJ/mol	Joback Method
hf	-834.10	kJ/mol	Joback Method
hfus	81.74	kJ/mol	Joback Method
hvap	122.34	kJ/mol	Joback Method
log10ws	-14.99		Crippen Method
logp	13.977		Crippen Method
mcvol	600.310	ml/mol	McGowan Method
pc	440.06	kPa	Joback Method
tb	1347.49	K	Joback Method
tc	1742.63	K	Joback Method
tf	321.10 ± 0.50	K	NIST Webbook
vc	2.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2700.18	J/mol×K	1347.49	Joback Method
cpg	2808.66	J/mol×K	1413.35	Joback Method
cpg	2929.52	J/mol×K	1479.20	Joback Method

cpg	3064.90	J/mol×K	1545.06	Joback Method
cpg	3216.92	J/mol×K	1610.92	Joback Method
cpg	3387.73	J/mol×K	1676.77	Joback Method
cpg	3579.45	J/mol×K	1742.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C303435&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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