

Cholesterol margarate

Other names:	(3«beta»)-cholest-5-en-3-yl heptadecanoate
Inchi:	InChI=1S/C44H78O2/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-42(45)46-37-29-31
InchiKey:	PPQNZVDOBYGOLY-KWDPNGDESA-N
Formula:	C44H78O2
SMILES:	CCCCCCCCCCCCCCCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCCC(C)C)C
Mol. weight [g/mol]:	639.09
CAS:	24365-37-5

Physical Properties

Property code	Value	Unit	Source
gf	249.52	kJ/mol	Joback Method
hf	-930.68	kJ/mol	Joback Method
hfus	78.95	kJ/mol	Joback Method
hvap	120.15	kJ/mol	Joback Method
log10ws	-14.71		Crippen Method
logp	13.811		Crippen Method
mcvol	590.520	ml/mol	McGowan Method
pc	448.30	kPa	Joback Method
tb	1320.45	K	Joback Method
tc	1701.43	K	Joback Method
tf	730.32	K	Joback Method
vc	2.279	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2626.41	J/molxK	1320.45	Joback Method
cpg	2722.28	J/molxK	1383.95	Joback Method
cpg	2827.91	J/molxK	1447.44	Joback Method
cpg	2945.10	J/molxK	1510.94	Joback Method
cpg	3075.70	J/molxK	1574.44	Joback Method
cpg	3221.51	J/molxK	1637.93	Joback Method
cpg	3384.36	J/molxK	1701.43	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C24365375&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
h vap:	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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