

Cholesteryl laurate

Other names:	5-Cholesten-3«beta»-ol laurate Cholesterol laurate Cholest-5-en-3-ol (3«beta»)-, dodecanoate Cholest-5-en-3«beta»-ol dodecanoate Cholesteryl dodecanoate Dodecanoic acid, cholesteryl ester 3«beta»-Dodecanoyloxycholest-5-ene cholest-5-en-3-«beta»-yl laurate
Inchi:	InChI=1S/C39H68O2/c1-7-8-9-10-11-12-13-14-15-19-37(40)41-32-24-26-38(5)31(28-32)
InchiKey:	RMLFYKFCGMSLTB-GKWGNEOISA-N
Formula:	C39H68O2
SMILES:	CCCCCCCCCCCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C
Mol. weight [g/mol]:	568.96
CAS:	1908-11-8

Physical Properties

Property code	Value	Unit	Source
gf	207.42	kJ/mol	Joback Method
hf	-827.48	kJ/mol	Joback Method
hfus	66.00	kJ/mol	Joback Method
hvap	109.02	kJ/mol	Joback Method
log10ws	-12.62		Crippen Method
logp	11.861		Crippen Method
mcvol	520.070	ml/mol	McGowan Method
pc	555.46	kPa	Joback Method
tb	1206.05	K	Joback Method
tc	1497.65	K	Joback Method
tf	364.00 ± 0.50	K	NIST Webbook
vc	1.998	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2195.39	J/mol×K	1206.05	Joback Method

cpg	2254.64	J/mol×K	1254.65	Joback Method
cpg	2317.66	J/mol×K	1303.25	Joback Method
cpg	2385.22	J/mol×K	1351.85	Joback Method
cpg	2458.09	J/mol×K	1400.45	Joback Method
cpg	2537.07	J/mol×K	1449.05	Joback Method
cpg	2622.91	J/mol×K	1497.65	Joback Method

Sources

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=C1908118&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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