

Cholest-5-en-3-ol (3«beta»)-, tetradecanoate

Other names:	Cholesterol, myristate Cholesteryl myristate Cholesteryl tetradecanoate Cholesteryl myristate 5-Cholesten-3«beta»-ol myristate cholest-5-en-3«beta»-yl myristate
Inchi:	InChI=1S/C41H72O2/c1-7-8-9-10-11-12-13-14-15-16-17-21-39(42)43-34-26-28-40(5)33(
InchiKey:	SJDMTGSQPOFVLR-UHFFFAOYSA-N
Formula:	C41H72O2
SMILES:	CCCCCCCCCCCCCCCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC3
Mol. weight [g/mol]:	597.01
CAS:	1989-52-2

Physical Properties

Property code	Value	Unit	Source
gf	224.26	kJ/mol	Joback Method
hf	-868.76	kJ/mol	Joback Method
hfus	71.18	kJ/mol	Joback Method
hvap	113.48	kJ/mol	Joback Method
log10ws	-13.46		Crippen Method
logp	12.641		Crippen Method
mcvol	548.250	ml/mol	McGowan Method
pc	508.41	kPa	Joback Method
tb	1251.81	K	Joback Method
tc	1573.12	K	Joback Method
tf	696.51	K	Joback Method
vc	2.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2363.30	J/mol×K	1251.81	Joback Method
cpg	2434.24	J/mol×K	1305.36	Joback Method
cpg	2510.64	J/mol×K	1358.91	Joback Method

cpg	2593.57	J/mol×K	1412.46	Joback Method
cpg	2684.08	J/mol×K	1466.01	Joback Method
cpg	2783.24	J/mol×K	1519.56	Joback Method
cpg	2892.11	J/mol×K	1573.12	Joback Method
hfust	46.69	kJ/mol	346.80	NIST Webbook
sfust	134.60	J/mol×K	346.80	NIST Webbook

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=C1989522&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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