

Cholesteryl stearate

Other names:	5-Cholesten-3«beta»-ol stearate Cholesterol stearate Cholest-5-en-3-ol (3«beta»)-, octadecanoate Cholesteryl octadecanoate Cholesteryl stearate 3«beta»-Octadecanoyloxycholest-5-ene cholest-5-en-3-«beta»-yl stearate
Inchi:	InChI=1S/C45H80O2/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-43(46)47-38-30
InchiKey:	XHRPOTDGOASDJS-LAQZWXCKSA-N
Formula:	C45H80O2
SMILES:	CCCCCCCCCCCCCCCCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCCC(C)C)C
Mol. weight [g/mol]:	653.12
CAS:	35602-69-8

Physical Properties

Property code	Value	Unit	Source
gf	257.94	kJ/mol	Joback Method
hf	-951.32	kJ/mol	Joback Method
hfus	81.54	kJ/mol	Joback Method
hvap	122.38	kJ/mol	Joback Method
log10ws	-15.13		Crippen Method
logp	14.201		Crippen Method
mvol	604.610	ml/mol	McGowan Method
pc	430.61	kPa	Joback Method
tb	1343.33	K	Joback Method
tc	1748.90	K	Joback Method
tf	741.59	K	Joback Method
vc	2.334	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2717.33	J/mol×K	1343.33	Joback Method
cpg	2824.12	J/mol×K	1410.93	Joback Method

cpg	2942.80	J/mol×K	1478.52	Joback Method
cpg	3075.60	J/mol×K	1546.12	Joback Method
cpg	3224.72	J/mol×K	1613.71	Joback Method
cpg	3392.40	J/mol×K	1681.31	Joback Method
cpg	3580.85	J/mol×K	1748.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35602698&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

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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