Lovastatin

Other names:

(S)-2-Methylbutyric acid, 8-ester with (4R,6R)-6-[2-[(1S,2S,6R,8S,8aR)-1,2,6,7,8,8a-hexahydro-8-hydroxy-2,6-dimethyl-1-naph
2-Methylbutanoic acid, (1S,3R,7S,8S,8aR)-1,2,3,7,8,8a-hexahydro-3,7-dimethyl-8-[2-[(2R,4R)-tetrahydro-4-hydr
6«alpha»-Methylcompactin ester (lovastatin)
6Â«alphaÂ»-Methylcompactin

8-[2-(4-Hydroxy-6-oxotetrahydro-2H-pyran-2-yl)ethyl]-3,7-dimethyl-(1S,3R,7S,8S,8aR)-1,
Altocor
2-methylbutanoate, (2S)-
Butanoic acid, 2-methyl-, (1S,3R,7S,8S,8aR)-1,2,3,7,8,8a-hexahydro-3,7-dimethyl-8-(2-((2R,4R)-tetrahydro-4-hydr
Butanoic acid, 2-methyl-, ester, [1S-[1«alpha»,3«alpha»,7«beta»,8«beta»(2S*,4S*),8a«beta»]]-1,2,3,7,8,8a-hexahydro-3,7-dimethyl-8-[2-(tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl)ethy
Butanoic acid, 2-methyl-, ester, 1S-[1«alpha»(R*),3«alpha»,7«beta»,8«beta»(2S*,4S*),8a«beta»]]-1,2,3,7,8,8a-hexahydro-3,7-dimethyl-8-[2-(tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl)ethy
Lovalip
MK-803
[1S-[1Â«alphaÂ»(R*),3Â«alphaÂ»,7Â«betaÂ»,8Â«betaÂ»(2S*,4S*),8aÂ«betaÂ»]]-
MSD 803
Mevacor
Mevinacor
Mevinolin
Mevlor
Monacolin K
Sivlor

Inchi: InChI=1S/C24H36O5/c1-5-15(3)24(27)29-21-11-14(2)10-17-7-6-16(4)20(23(17)21)9-8-19

InchiKey: PCZOHLXUXFIOCF-UHFFFAOYSA-N

Formula: C24H36O5

SMILES: CCC(C)C(=O)OC1CC(C)C=C2C=CC(C)C(CCC3CC(O)CC(=O)O3)C21

Mol. weight [g/mol]: 404.54

CAS: 75330-75-5

Physical Properties

Property code	Value	Unit	Source
gf	-313.69	kJ/mol	Joback Method
hf	-1012.69	kJ/mol	Joback Method
hfus	54.80	kJ/mol	Joback Method
hvap	104.17	kJ/mol	Joback Method
log10ws	-6.01		Aqueous Solubility Prediction Method
log10ws	-6.00		Estimated Solubility Method
logp	4.196		Crippen Method
mcvol	328.590	ml/mol	McGowan Method

pc	1222.55	kPa	Joback Method
tb	1046.05	K	Joback Method
tc	1282.23	K	Joback Method
tf	452.15	K	Solubility of Lovastatin in Acetone + Water Solvent Mixtures
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1234.29	J/mol×K	1046.05	Joback Method
cpg	1247.72	J/mol×K	1085.41	Joback Method
cpg	1258.79	J/mol×K	1124.78	Joback Method
cpg	1267.52	J/mol×K	1164.14	Joback Method
cpg	1273.93	J/mol×K	1203.50	Joback Method
cpg	1278.03	J/mol×K	1242.86	Joback Method
cpg	1279.86	J/mol×K	1282.23	Joback Method
hfust	43.14	kJ/mol	445.50	NIST Webbook
hfust	36.53	kJ/mol	444.30	NIST Webbook

Sources

Solubility of Simvastatin and Lovastatin in Mixtures of Dichloromethane and Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je700019h
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Solubility of Lovastatin in Acetone + Water Solvent Mixtures:	https://www.doi.org/10.1021/je800063d
Solubility of Lovastatin in Acetone, Methanol, Ethanol, Ethyl Acetate, and Butyl Acetate between 283 K and 323 K:	https://www.doi.org/10.1021/je0500781
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility of Lovastatin in Ethyl Acetate, Propyl Acetate, Isopropyl Acetate, Butyl Acetate, sec-Butyl Acetate, Isobutyl Acetate, tert-Butyl Acetate, and 2-Butanone, between (285 and 313) K:	https://www.doi.org/10.1021/je800120p
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75330755&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume