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)
	8-[2-(4-Hydroxy-6-oxotetrahydro-2H-pyran-2-yl)ethyl]-3,7-dimethyl-(1S,3R,7S,8S,8aR)-1,
	Alfocor
	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»]]-
	[1S-[1«alpha»,3«alpha»,7«beta»,8«beta»(2S*,4S*),8a«beta»]]-2,3,7,8,8a-hexahydro-3,7-dimethyl-8-[2-(tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl)ethy
	Lovalip
	MK-803
	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]:	404.55

Physical Properties

Property code	Value	Unit	Source
hfus	54.80	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
tf	452.15	K	Solubility of Lovastatin in Acetone + Water Solvent Mixtures

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

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Cheméo Relay (1.0):	
Solubility of Simvastatin and Lovastatin in Mixtures of Dichloromethane and Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je700019h
Solubility of Lovastatin in Acetone + Water Solvent Mixtures:	https://www.doi.org/10.1021/je800063d
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75330755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0, beta):	
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
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

tf: Normal melting (fusion) point