Simvastatin

Other names:	(+)-Simvastatin 2,2-Dimethylbutanoic acid, (1S,3R,7S,8S,8aR)-1,2,3,7,8,8a-hexahydro-3,7-dimethyl-8-[2-[(2R,4R)-tetrahydro-4-hydro 2,2-Dimethylbutyric 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 Butanoic acid, 2,2-dimethyl-, 1,2,3,7,8,8a-hexahydro-3,7-dimethyl-8-[2-(tetrahydro-4-hydroxy-6-oxo-2H-pyran-2yl)-ethy Butanoic acid, 2,2-dimethyl-, 1,2,3,7,8,8a-hexahydro-3,7-dimethyl-8-[2-(tetrahydro-4-hydroxy-6-oxo-2H-pyran-2yl)-ethy Butanoic acid, 2,2-dimethyl-, 1S-[1Â«alphaÂ»,3Â«alphaÂ», 7Â«betaÂ», 8Â«betaÂ»-(2S*, 4S*), 8a Butanoic acid, 2,2-dimethyl-, (1S,3R,7S,8S,8aR)-1,2,3,7,8,8a-hexahydro-3,7-dimethyl-8-[2-[(2R,4R)-tetrahydro-4-hydro Butanoic acid, 2,2-dimethyl-, 1,2,3,7,8,8a-hexahydro-3,7-dimethyl-8-[2-(tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl)ethy Butanoic acid, 2,2-dimethyl-, 1,2,3,7,8,8a-hexahydro-3,7-dimethyl-8-[2-(tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl)ethy Synvinolin Zocor
Inchi:	InChI=1S/C25H38O5/c1-6-25(4,5)24(28)30-21-12-15(2)11-17-8-7-16(3)20(23(17)21)10-9
InchiKey:	RYMZZMVNJRMUDD-UHFFFAOYSA-N
Formula:	C25H38O5
SMILES:	CCC(C)(C)C(=O)OC1CC(C)C=C2C=CC(C)C(CCC3CC(O)CC(=O)O3)C21
Mol. weight [g/mol]:	418.57
CAS:	79902-63-9

Physical Properties

Property code	Value	Unit	Source
gf	-299.99	kJ/mol	Joback Method
hf	-1036.80	kJ/mol	Joback Method
hfus	32.17	kJ/mol	Solubility and limiting activity coefficient of simvastatin in different organic solvents
hfus	30.13	kJ/mol	Solution thermodynamics of simvastatin in pure solvents and binary solvent mixtures
hvap	105.49	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.586		Crippen Method
mcvol	342.680	ml/mol	McGowan Method
pc	1153.00	kPa	Joback Method
rinpol	3221.90		NIST Webbook
tb	1066.14	K	Joback Method
tc	1306.44	K	Joback Method
tf	627.96	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1295.56	J/mol×K	1066.14	Joback Method
cpg	1309.14	J/mol×K	1106.19	Joback Method
cpg	1320.46	J/mol×K	1146.24	Joback Method
cpg	1329.58	J/mol×K	1186.29	Joback Method
cpg	1336.56	J/mol×K	1226.34	Joback Method
cpg	1341.45	J/mol×K	1266.39	Joback Method
cpg	1344.31	J/mol×K	1306.44	Joback Method

Sources

Solubility and limiting activity coefficient of simvastatin in different organic solvents:	https://www.doi.org/10.1016/j.fluid.2009.03.006
Solution thermodynamics of simvastatin in pure solvents and binary solvent mixtures:	https://www.doi.org/10.1016/j.fluid.2015.07.055
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79902639&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume